NMR Frequency Tables

NMR Frequencies vs. Bruker Field Strengths – sorted by increasing atomic number

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
1	H	1/2	99.9885	5.87E+03	**1.00E+00**	**300.130**	**400.130**	**500.130**	**600.130**	**700.130**	**750.130**	**800.130**	**850.130**	**900.130**	**950.130**	**1000.130**
2	H	1	0.0115	6.52E−03	9.65E−03	46.072	61.422	76.773	92.124	107.474	115.150	122.825	130.500	138.175	145.851	153.526
3	H	1/2		-	1.21E+00	320.131	426.795	533.459	640.123	746.786	800.118	853.450	906.782	960.114	1013.446	1066.778
3	He	1/2	1.34E-04	3.48E−03	4.42E−01	228.636	304.815	380.994	457.173	533.352	571.441	609.531	647.620	685.710	723.799	761.889
6	Li	1	7.59	3.79E+00	8.50E−03	44.167	58.883	73.600	88.316	103.032	110.390	117.748	125.106	132.464	139.822	147.180
7	Li	3/2	92.41	1.59E+03	2.94E−01	116.642	155.506	194.370	233.233	272.097	291.529	310.961	330.393	349.825	369.257	388.688
9	Be	3/2	100.0	8.15E+01	1.39E−02	42.174	56.226	70.277	84.329	98.381	105.407	112.433	119.459	126.485	133.510	140.536
10	B	3	19.9	2.32E+01	1.99E−02	32.245	42.989	53.732	64.476	75.220	80.591	85.963	91.335	96.707	102.079	107.451
11	B	3/2	80.1	7.77E+02	1.65E−01	96.294	128.378	160.462	192.546	224.630	240.672	256.714	272.755	288.797	304.839	320.881
13	C	1/2	1.07	**1.00E+00**	1.59E−02	75.468	100.613	125.758	150.903	176.048	188.620	201.193	213.765	226.338	238.910	251.483
14	N	1	99.636	5.90E+00	1.01E−03	21.688	28.915	36.141	43.367	50.594	54.207	57.820	61.433	65.046	68.659	72.273
15	N	1/2	0.364	2.23E−02	1.04E−03	30.423	40.560	50.697	60.834	70.971	76.039	81.107	86.176	91.244	96.312	101.381
17	O	5/2	0.038	6.50E−02	2.91E−02	40.687	54.243	67.800	81.356	94.913	101.691	108.469	115.248	122.026	128.804	135.582
19	F	1/2	100.0	4.89E+03	8.32E−01	282.404	376.498	470.592	564.686	658.780	705.827	752.874	799.921	846.968	894.015	941.062
21	Ne	3/2	0.27	3.91E−02	2.46E−03	23.693	31.587	39.482	47.376	55.270	59.217	63.165	67.112	71.059	75.006	78.953
23	Na	3/2	100.0	5.45E+02	9.27E−02	79.390	105.842	132.294	158.746	185.198	198.424	211.650	224.876	238.101	251.327	264.553
25	Mg	5/2	10.00	1.58E+00	2.68E−03	18.373	24.494	30.616	36.738	42.859	45.920	48.981	52.042	55.103	58.163	61.224
27	Al	5/2	100.0	1.22E+03	2.07E−01	78.204	104.261	130.318	156.375	182.432	195.460	208.489	221.517	234.546	247.574	260.602
29	Si	1/2	4.685	2.16E+00	7.86E−03	59.627	79.495	99.362	119.229	139.096	149.030	158.963	168.897	178.831	188.764	198.698
31	P	1/2	100.0	3.91E+02	6.65E−02	121.495	161.976	202.457	242.938	283.419	303.659	323.900	344.140	364.380	384.621	404.861
33	S	3/2	0.75	1.00E−01	2.27E−03	23.038	30.714	38.390	46.066	53.742	57.580	61.418	65.256	69.094	72.932	76.770
35	Cl	3/2	75.76	2.10E+01	4.72E−03	29.406	39.204	49.002	58.800	68.598	73.497	78.396	83.295	88.194	93.093	97.992
37	Cl	3/2	24.24	3.88E+00	2.72E−03	24.478	32.634	40.789	48.945	57.101	61.179	65.256	69.334	73.412	77.490	81.568
39	K	3/2	93.258	2.79E+00	5.10E−04	14.005	18.672	23.338	28.004	32.671	35.004	37.337	39.670	42.003	44.337	46.670
41	K	3/2	6.730	3.34E−02	8.44E−05	7.687	10.249	12.810	15.371	17.932	19.213	20.494	21.774	23.055	24.336	25.616
43	Ca	7/2	0.135	5.10E−02	6.43E−03	20.199	26.929	33.659	40.389	47.119	50.484	53.849	57.214	60.579	63.944	67.309
45	Sc	7/2	100.0	1.78E+03	3.02E−01	72.907	97.199	121.490	145.782	170.074	182.220	194.366	206.511	218.657	230.803	242.949
47	Ti	5/2	7.44	9.18E−01	2.10E−03	16.920	22.557	28.195	33.833	39.470	42.289	45.108	47.926	50.745	53.564	56.383
49	Ti	7/2	5.41	1.20E+00	3.78E−03	16.924	22.563	28.203	33.842	39.481	42.300	45.120	47.939	50.759	53.578	56.398
50	V	6	0.250	8.18E−01	5.57E−02	29.924	39.894	49.865	59.835	69.805	74.790	79.775	84.761	89.746	94.731	99.716
51	V	7/2	99.750	2.25E+03	3.84E−01	78.943	105.246	131.549	157.852	184.155	197.306	210.458	223.609	236.761	249.912	263.064
53	Cr	3/2	9.501	5.07E−01	9.08E−04	16.965	22.617	28.270	33.922	39.575	42.401	45.227	48.054	50.880	53.706	56.532
55	Mn	5/2	100.0	1.05E+03	1.79E−01	74.400	99.189	123.978	148.768	173.557	185.951	198.346	210.741	223.135	235.530	247.924
57	Fe	1/2	2.119	4.25E−03	3.42E−05	9.718	12.955	16.193	19.431	22.669	24.288	25.906	27.525	29.144	30.763	32.382
59	Co	7/2	100.0	1.64E+03	2.78E−01	71.212	94.939	118.666	142.393	166.120	177.984	189.847	201.711	213.575	225.438	237.302
61	Ni	3/2	1.1399	2.40E−01	3.59E−03	26.820	35.756	44.692	53.628	62.564	67.032	71.500	75.968	80.436	84.904	89.372
63	Cu	3/2	69.15	3.82E+02	9.39E−02	79.581	106.096	132.612	159.127	185.643	198.901	212.158	225.416	238.674	251.931	265.189
65	Cu	3/2	30.85	2.08E+02	1.15E−01	85.248	113.652	142.055	170.459	198.863	213.065	227.266	241.468	255.670	269.872	284.074
67	Zn	5/2	4.102	6.92E−01	2.87E−03	18.779	25.035	31.292	37.549	43.806	46.934	50.063	53.191	56.319	59.448	62.576
69	Ga	3/2	60.108	2.46E+02	6.97E−02	72.035	96.037	120.038	144.039	168.041	180.041	192.042	204.043	216.043	228.044	240.045
71	Ga	3/2	39.892	3.35E+02	1.43E−01	91.530	122.026	152.523	183.020	213.517	228.765	244.013	259.262	274.510	289.758	305.007

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
73	Ge	9/2	7.76	6.44E−01	1.41E−03	10.469	13.958	17.446	20.934	24.423	26.167	27.911	29.655	31.399	33.144	34.888
75	As	3/2	100.0	1.49E+02	2.54E−02	51.390	68.513	85.635	102.758	119.881	128.442	137.003	145.564	154.126	162.687	171.248
77	Se	1/2	7.63	3.15E+00	7.03E−03	57.239	76.311	95.382	114.454	133.525	143.061	152.597	162.133	171.668	181.204	190.740
79	Br	3/2	50.69	2.37E+02	7.94E−02	75.195	100.248	125.302	150.356	175.410	187.937	200.464	212.991	225.518	238.045	250.572
81	Br	3/2	49.31	2.88E+02	9.95E−02	81.055	108.061	135.068	162.074	189.081	202.584	216.087	229.591	243.094	256.597	270.100
83	Kr	9/2	11.500	1.28E+00	1.90E−03	11.548	15.395	19.243	23.091	26.938	28.862	30.786	32.710	34.633	36.557	38.481
85	Rb	5/2	72.17	4.50E+01	1.06E−02	28.977	38.632	48.287	57.942	67.597	72.425	77.252	82.080	86.907	91.735	96.562
87	Rb	3/2	27.83	2.90E+02	1.77E−01	98.204	130.924	163.645	196.365	229.086	245.446	261.806	278.166	294.527	310.887	327.247
87	Sr	9/2	7.00	1.12E+00	2.72E−03	13.007	17.341	21.675	26.009	30.342	32.509	34.676	36.843	39.010	41.177	43.344
89	Y	1/2	100.0	7.00E−01	1.19E−04	14.707	19.607	24.507	29.408	34.308	36.758	39.208	41.658	44.108	46.558	49.008
91	Zr	5/2	11.22	6.26E+00	9.49E−03	27.901	37.197	46.494	55.790	65.086	69.734	74.382	79.031	83.679	88.327	92.975
93	Nb	9/2	100.0	2.87E+03	4.88E−01	73.460	97.936	122.413	146.889	171.365	183.603	195.841	208.079	220.317	232.555	244.794
95	Mo	5/2	15.90	3.06E+00	3.27E−03	19.559	26.076	32.593	39.110	45.627	48.885	52.144	55.402	58.661	61.919	65.178
97	Mo	5/2	9.56	1.96E+00	3.49E−03	19.970	26.623	33.277	39.931	46.585	49.911	53.238	56.565	59.892	63.219	66.546
99	Tc	9/2		-	3.82E−01	67.554	90.063	112.571	135.079	157.588	168.842	180.096	191.350	202.604	213.858	225.113
99	Ru	5/2	12.76	8.46E−01	1.13E−03	13.821	18.427	23.032	27.637	32.242	34.545	36.847	39.150	41.452	43.755	46.057
101	Ru	5/2	17.06	1.58E+00	1.57E−03	15.491	20.652	25.814	30.975	36.136	38.717	41.298	43.878	46.459	49.040	51.620
103	Rh	1/2	100.0	1.86E−01	3.17E−05	9.563	12.750	15.936	19.123	22.309	23.902	25.496	27.089	28.682	30.275	31.869
105	Pd	5/2	22.33	1.49E+00	1.13E−03	13.734	18.310	22.886	27.463	32.039	34.327	36.615	38.903	41.191	43.479	45.767
107	Ag	1/2	51.839	2.05E−01	6.74E−05	12.149	16.197	20.244	24.292	28.340	30.364	32.388	34.412	36.436	38.460	40.483
109	Ag	1/2	48.161	2.90E−01	1.02E−04	13.967	18.620	23.274	27.927	32.581	34.908	37.234	39.561	41.888	44.215	46.541
111	Cd	1/2	12.80	7.27E+00	9.66E−03	63.674	84.890	106.105	127.320	148.536	159.144	169.751	180.359	190.967	201.575	212.182
113	Cd	1/2	12.22	7.94E+00	1.11E−02	66.608	88.802	110.995	133.188	155.381	166.478	177.574	188.671	199.767	210.864	221.961
113	In	9/2	4.29	8.85E+01	3.51E−01	65.626	87.491	109.357	131.223	153.089	164.022	174.954	185.887	196.820	207.753	218.686
115	In	9/2	95.71	1.99E+03	3.53E−01	65.766	87.679	109.592	131.504	153.417	164.373	175.330	186.286	197.242	208.198	219.155
115	Sn	1/2	0.34	7.11E−01	3.56E−02	98.199	130.918	163.636	196.355	229.074	245.433	261.793	278.152	294.511	310.871	327.230
117	Sn	1/2	7.68	2.08E+01	4.60E−02	106.943	142.575	178.208	213.840	249.472	267.288	285.104	302.921	320.737	338.553	356.369
119	Sn	1/2	8.59	2.66E+01	5.27E−02	111.920	149.211	186.502	223.792	261.083	279.728	298.374	317.019	335.664	354.309	372.955
121	Sb	5/2	57.21	5.48E+02	1.63E−01	71.823	95.753	119.684	143.615	167.545	179.510	191.476	203.441	215.406	227.372	239.337
123	Sb	7/2	42.79	1.17E+02	4.66E−02	38.894	51.854	64.813	77.772	90.731	97.211	103.691	110.170	116.650	123.129	129.609
123	Te	1/2	0.89	9.61E−01	1.84E−02	78.543	104.713	130.883	157.052	183.222	196.307	209.392	222.477	235.562	248.647	261.731
125	Te	1/2	7.07	1.34E+01	3.22E−02	94.690	126.240	157.790	189.340	220.889	236.664	252.439	268.214	283.989	299.764	315.539
127	I	5/2	100.0	5.60E+02	9.54E−02	60.048	80.056	100.063	120.071	140.078	150.082	160.086	170.090	180.093	190.097	200.101
129	Xe	1/2	26.4006	3.35E+01	2.16E−02	83.467	111.277	139.087	166.897	194.707	208.613	222.518	236.423	250.328	264.233	278.138
131	Xe	3/2	21.2324	3.51E+00	2.82E−03	24.742	32.986	41.230	49.474	57.718	61.840	65.962	70.084	74.206	78.328	82.450
133	Cs	7/2	100.0	2.84E+02	4.84E−02	39.365	52.482	65.598	78.714	91.830	98.388	104.946	111.504	118.062	124.620	131.178
135	Ba	3/2	6.592	1.94E+00	5.01E−03	29.816	39.751	49.685	59.620	69.554	74.521	79.489	84.456	89.423	94.390	99.357
137	Ba	3/2	11.232	4.62E+00	7.00E−03	33.353	44.466	55.579	66.692	77.805	83.361	88.918	94.474	100.031	105.587	111.144
138	La	5	0.090	4.97E−01	9.40E−02	39.600	52.794	65.989	79.183	92.377	98.974	105.572	112.169	118.766	125.363	131.960
139	La	7/2	99.910	3.56E+02	6.06E−02	42.395	56.521	70.647	84.772	98.898	105.961	113.023	120.086	127.149	134.212	141.275
141	Pr	5/2	100.0	1.97E+03	3.35E−01	91.89	122.51	153.12	183.74	214.36	229.67	244.97	260.28	275.59	290.90	306.21

NMR Frequency Tables

NMR Frequencies vs. Bruker Field Strengths – sorted by increasing atomic number

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
143	Nd	7/2	12.2	2.43E+00	3.39E−03	16.35	21.80	27.25	32.69	38.14	40.86	43.59	46.31	49.04	51.76	54.48
145	Nd	7/2	8.3	3.87E−01	7.93E−04	10.07	13.43	16.78	20.14	23.49	25.17	26.85	28.53	30.20	31.88	33.56
147	Sm	7/2	14.99	1.34E+00	1.52E−03	12.51	16.68	20.84	25.01	29.18	31.26	33.35	35.43	37.52	39.60	41.68
149	Sm	7/2	13.82	6.92E−01	8.52E−04	10.31	13.75	17.18	20.62	24.06	25.77	27.49	29.21	30.93	32.64	34.36
151	Eu	5/2	47.81	5.04E+02	1.79E−01	74.62	99.48	124.34	149.20	174.06	186.49	198.92	211.35	223.78	236.22	248.65
153	Eu	5/2	52.19	4.73E+01	1.54E−02	32.94	43.91	54.88	65.86	76.83	82.32	87.80	93.29	98.78	104.26	109.75
155	Gd	3/2	14.80	1.26E−01	1.45E−04	9.21	12.28	15.35	18.42	21.49	23.03	24.56	26.10	27.63	29.17	30.70
157	Gd	3/2	15.65	3.00E−01	3.26E−04	12.08	16.11	20.13	24.16	28.19	30.20	32.21	34.22	36.24	38.25	40.26
159	Tb	3/2	100.0	4.08E+02	6.94E−02	72.14	96.18	120.22	144.26	168.29	180.31	192.33	204.35	216.37	228.39	240.41
161	Dy	5/2	18.889	5.26E−01	4.74E−04	10.32	13.75	17.19	20.63	24.07	25.78	27.50	29.22	30.94	32.66	34.38
163	Dy	5/2	24.896	1.91E+00	1.31E−03	14.46	19.28	24.10	28.92	33.74	36.15	38.56	40.97	43.38	45.79	48.20
165	Ho	7/2	100.0	1.16E+03	1.98E−01	63.43	84.57	105.71	126.84	147.98	158.54	169.11	179.68	190.25	200.82	211.38
167	Er	7/2	22.869	6.77E−01	5.04E−04	8.66	11.54	14.42	17.31	20.19	21.63	23.08	24.52	25.96	27.40	28.85
169	Tm	1/2	100.0	3.32E+00	5.66E−04	24.82	33.10	41.37	49.64	57.91	62.04	66.18	70.32	74.45	78.59	82.72
171	Yb	1/2	14.28	4.63E+00	5.52E−03	52.521	70.020	87.519	105.019	122.518	131.268	140.017	148.767	157.517	166.266	175.016
173	Yb	5/2	16.13	1.28E+00	1.35E−03	14.61	19.48	24.35	29.22	34.09	36.52	38.96	41.39	43.83	46.26	48.69
175	Lu	7/2	97.41	1.79E+02	3.13E−02	34.27	45.69	57.11	68.53	79.94	85.65	91.36	97.07	102.78	108.49	114.20
176	Lu	7	2.59	6.05E+00	3.98E−02	24.33	32.43	40.53	48.64	56.74	60.80	64.85	68.90	72.95	77.01	81.06
177	Hf	7/2	18.60	1.53E+00	1.40E−03	12.18	16.24	20.30	24.36	28.42	30.45	32.48	34.51	36.53	38.56	40.59
179	Hf	9/2	13.62	4.38E−01	5.47E−04	7.65	10.20	12.75	15.30	17.85	19.13	20.40	21.68	22.95	24.23	25.50
181	Ta	7/2	99.988	2.20E+02	3.74E−02	35.984	47.974	59.964	71.953	83.943	89.938	95.932	101.927	107.922	113.917	119.912
183	W	1/2	14.31	6.31E−02	7.50E−05	12.505	16.671	20.837	25.004	29.170	31.253	33.337	35.420	37.503	39.586	41.669
185	Re	5/2	37.40	3.05E+02	1.39E−01	67.603	90.128	112.652	135.177	157.701	168.964	180.226	191.488	202.751	214.013	225.275
187	Re	5/2	62.60	5.26E+02	1.43E−01	68.284	91.036	113.788	136.539	159.291	170.667	182.042	193.418	204.794	216.170	227.546
187	Os	1/2	1.96	1.43E−03	1.24E−05	6.850	9.132	11.415	13.697	15.979	17.120	18.262	19.403	20.544	21.685	22.826
189	Os	3/2	16.15	2.32E+00	2.44E−03	23.306	31.072	38.837	46.602	54.368	58.251	62.133	66.016	69.899	73.781	77.664
191	Ir	3/2	37.3	6.38E−02	2.91E−05	5.40	7.20	9.00	10.79	12.59	13.49	14.39	15.29	16.19	17.09	17.99
193	Ir	3/2	62.7	1.37E−01	3.73E−05	5.86	7.82	9.77	11.73	13.68	14.66	15.63	16.61	17.59	18.56	19.54
195	Pt	1/2	33.832	2.07E+01	1.04E−02	64.518	86.015	107.512	129.009	150.505	161.254	172.002	182.751	193.499	204.247	214.996
197	Au	3/2	100.0	1.62E−01	2.76E−05	5.31	7.08	8.84	10.61	12.38	13.26	14.15	15.03	15.92	16.80	17.69
199	Hg	1/2	16.87	5.89E+00	5.94E−03	53.756	71.667	89.577	107.488	125.399	134.354	143.310	152.265	161.221	170.176	179.132
201	Hg	3/2	13.18	1.16E+00	1.49E−03	19.843	26.455	33.067	39.678	46.290	49.595	52.901	56.207	59.513	62.819	66.124
203	Tl	1/2	29.52	3.40E+02	1.96E−01	171.444	228.567	285.690	342.813	399.937	428.498	457.060	485.621	514.183	542.745	571.306
205	Tl	1/2	70.48	8.36E+02	2.02E−01	173.127	230.810	288.494	346.178	403.862	432.704	461.546	490.388	519.230	548.071	576.913
207	Pb	1/2	22.1	1.18E+01	9.06E−03	62.789	83.710	104.630	125.551	146.471	156.932	167.392	177.852	188.313	198.773	209.233
209	Bi	9/2	100.0	8.48E+02	1.44E−01	48.229	64.298	80.367	96.437	112.506	120.541	128.575	136.610	144.644	152.679	160.714
209	Po	1/2		-	1.44E−02	73.08	97.42	121.77	146.12	170.47	182.64	194.81	206.99	219.16	231.34	243.51
231	Pa	3/2	100.0	4.06E+02	6.90E−02	72.00	95.99	119.98	143.97	167.96	179.96	191.95	203.94	215.94	227.93	239.93
235	U	7/2	0.7204	6.53E−03	1.54E−04	5.527	7.368	9.209	11.051	12.892	13.813	14.734	15.654	16.575	17.496	18.416

NMR Frequencies vs. Bruker Field Strengths – sorted with decreasing Larmor frequency

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
3	H	1/2		–	1.21E+00	320.131	426.795	533.459	640.123	746.786	800.118	853.450	906.782	960.114	1013.446	1066.778
1	H	1/2	99.9885	5.87E+03	**1.00E+00**	**300.130**	**400.130**	**500.130**	**600.130**	**700.130**	**750.130**	**800.130**	**850.130**	**900.130**	**950.130**	**1000.130**
19	F	1/2	100.0	4.89E+03	8.32E–01	282.404	376.498	470.592	564.686	658.780	705.827	752.874	799.921	846.968	894.015	941.062
3	He	1/2	1.34E–04	3.48E–03	4.42E–01	228.636	304.815	380.994	457.173	533.352	571.441	609.531	647.620	685.710	723.799	761.889
205	Tl	1/2	70.48	8.36E+02	2.02E–01	173.127	230.810	288.494	346.178	403.862	432.704	461.546	490.388	519.230	548.071	576.913
203	Tl	1/2	29.52	3.40E+02	1.96E–01	171.444	228.567	285.690	342.813	399.937	428.498	457.060	485.621	514.183	542.745	571.306
31	P	1/2	100.0	3.91E+02	6.65E–02	121.495	161.976	202.457	242.938	283.419	303.659	323.900	344.140	364.380	384.621	404.861
7	Li	3/2	92.41	1.59E+03	2.94E–01	116.642	155.506	194.370	233.233	272.097	291.529	310.961	330.393	349.825	369.257	388.688
119	Sn	1/2	8.59	2.66E+01	5.27E–02	111.920	149.211	186.502	223.792	261.083	279.728	298.374	317.019	335.664	354.309	372.955
117	Sn	1/2	7.68	2.08E+01	4.60E–02	106.943	142.575	178.208	213.840	249.472	267.288	285.104	302.921	320.737	338.553	356.369
87	Rb	3/2	27.83	2.90E+02	1.77E–01	98.204	130.924	163.645	196.365	229.086	245.446	261.806	278.166	294.527	310.887	327.247
115	Sn	1/2	0.34	7.11E–01	3.56E–02	98.199	130.918	163.636	196.355	229.074	245.433	261.793	278.152	294.511	310.871	327.230
11	B	3/2	80.1	7.77E+02	1.65E–01	96.294	128.378	160.462	192.546	224.630	240.672	256.714	272.755	288.797	304.839	320.881
125	Te	1/2	7.07	1.34E+01	3.22E–02	94.690	126.240	157.790	189.340	220.889	236.664	252.439	268.214	283.989	299.764	315.539
141	Pr	5/2	100.0	1.97E+03	3.35E–01	91.89	122.51	153.12	183.74	214.36	229.67	244.97	260.28	275.59	290.90	306.21
71	Ga	3/2	39.892	3.35E+02	1.43E–01	91.530	122.026	152.523	183.020	213.517	228.765	244.013	259.262	274.510	289.758	305.007
65	Cu	3/2	30.85	2.08E+02	1.15E–01	85.248	113.652	142.055	170.459	198.863	213.065	227.266	241.468	255.670	269.872	284.074
129	Xe	1/2	26.4006	3.35E+01	2.16E–02	83.467	111.277	139.087	166.897	194.707	208.613	222.518	236.423	250.328	264.233	278.138
81	Br	3/2	49.31	2.88E+02	9.95E–02	81.055	108.061	135.068	162.074	189.081	202.584	216.087	229.591	243.094	256.597	270.100
63	Cu	3/2	69.15	3.82E+02	9.39E–02	79.581	106.096	132.612	159.127	185.643	198.901	212.158	225.416	238.674	251.931	265.189
23	Na	3/2	100.0	5.45E+02	9.27E–02	79.390	105.842	132.294	158.746	185.198	198.424	211.650	224.876	238.101	251.327	264.553
51	V	7/2	99.750	2.25E+03	3.84E–01	78.943	105.246	131.549	157.852	184.155	197.306	210.458	223.609	236.761	249.912	263.064
123	Te	1/2	0.89	9.61E–01	1.84E–02	78.543	104.713	130.883	157.052	183.222	196.307	209.392	222.477	235.562	248.647	261.731
27	Al	5/2	100.0	1.22E+03	2.07E–01	78.204	104.261	130.318	156.375	182.432	195.460	208.489	221.517	234.546	247.574	260.602
13	C	1/2	1.07	**1.00E+00**	1.59E–02	75.468	100.613	125.758	150.903	176.048	188.620	201.193	213.765	226.338	238.910	251.483
79	Br	3/2	50.69	2.37E+02	7.94E–02	75.195	100.248	125.302	150.356	175.410	187.937	200.464	212.991	225.518	238.045	250.572
151	Eu	5/2	47.81	5.04E+02	1.79E–01	74.62	99.48	124.34	149.20	174.06	186.49	198.92	211.35	223.78	236.22	248.65
55	Mn	5/2	100.0	1.05E+03	1.79E–01	74.400	99.189	123.978	148.768	173.557	185.951	198.346	210.741	223.135	235.530	247.924
93	Nb	9/2	100.0	2.87E+03	4.88E–01	73.460	97.936	122.413	146.889	171.365	183.603	195.841	208.079	220.317	232.555	244.794
209	Po	1/2		–	1.44E–02	73.08	97.42	121.77	146.12	170.47	182.64	194.81	206.99	219.16	231.34	243.51
45	Sc	7/2	100.0	1.78E+03	3.02E–01	72.907	97.199	121.490	145.782	170.074	182.220	194.366	206.511	218.657	230.803	242.949
159	Tb	3/2	100.0	4.08E+02	6.94E–02	72.14	96.18	120.22	144.26	168.29	180.31	192.33	204.35	216.37	228.39	240.41
69	Ga	3/2	60.108	2.46E+02	6.97E–02	72.035	96.037	120.038	144.039	168.041	180.041	192.042	204.043	216.043	228.044	240.045
231	Pa	3/2	100.0	4.06E+02	6.90E–02	72.00	95.99	119.98	143.97	167.96	179.96	191.95	203.94	215.94	227.93	239.93
121	Sb	5/2	57.21	5.48E+02	1.63E–01	71.823	95.753	119.684	143.615	167.545	179.510	191.476	203.441	215.406	227.372	239.337
59	Co	7/2	100.0	1.64E+03	2.78E–01	71.212	94.939	118.666	142.393	166.120	177.984	189.847	201.711	213.575	225.438	237.302
187	Re	5/2	62.60	5.26E+02	1.43E–01	68.284	91.036	113.788	136.539	159.291	170.667	182.042	193.418	204.794	216.170	227.546
185	Re	5/2	37.40	3.05E+02	1.39E–01	67.603	90.128	112.652	135.177	157.701	168.964	180.226	191.488	202.751	214.013	225.275
99	Tc	9/2		–	3.82E–01	67.554	90.063	112.571	135.079	157.588	168.842	180.096	191.350	202.604	213.858	225.113
113	Cd	1/2	12.22	7.94E+00	1.11E–02	66.608	88.802	110.995	133.188	155.381	166.478	177.574	188.671	199.767	210.864	221.961
115	In	9/2	95.71	1.99E+03	3.53E–01	65.766	87.679	109.592	131.504	153.417	164.373	175.330	186.286	197.242	208.198	219.155

NMR Frequency Tables

NMR Frequencies vs. Bruker Field Strengths – sorted with decreasing Larmor frequency

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
113	In	9/2	4.29	8.85E+01	3.51E–01	65.626	87.491	109.357	131.223	153.089	164.022	174.954	185.887	196.820	207.753	218.686
195	Pt	1/2	33.832	2.07E+01	1.04E–02	64.518	86.015	107.512	129.009	150.505	161.254	172.002	182.751	193.499	204.247	214.996
111	Cd	1/2	12.80	7.27E+00	9.66E–03	63.674	84.890	106.105	127.320	148.536	159.144	169.751	180.359	190.967	201.575	212.182
165	Ho	7/2	100.0	1.16E+03	1.98E–01	63.43	84.57	105.71	126.84	147.98	158.54	169.11	179.68	190.25	200.82	211.38
207	Pb	1/2	22.1	1.18E+01	9.06E–03	62.789	83.710	104.630	125.551	146.471	156.932	167.392	177.852	188.313	198.773	209.233
127	I	5/2	100.0	5.60E+02	9.54E–02	60.048	80.056	100.063	120.071	140.078	150.082	160.086	170.090	180.093	190.097	200.101
29	Si	1/2	4.685	2.16E+00	7.86E–03	59.627	79.495	99.362	119.229	139.096	149.030	158.963	168.897	178.831	188.764	198.698
77	Se	1/2	7.63	3.15E+00	7.03E–03	57.239	76.311	95.382	114.454	133.525	143.061	152.597	162.133	171.668	181.204	190.740
199	Hg	1/2	16.87	5.89E+00	5.94E–03	53.756	71.667	89.577	107.488	125.399	134.354	143.310	152.265	161.221	170.176	179.132
171	Yb	1/2	14.28	4.63E+00	5.52E–03	52.521	70.020	87.519	105.019	122.518	131.268	140.017	148.767	157.517	166.266	175.016
75	As	3/2	100.0	1.49E+02	2.54E–02	51.390	68.513	85.635	102.758	119.881	128.442	137.003	145.564	154.126	162.687	171.248
209	Bi	9/2	100.0	8.48E+02	1.44E–01	48.229	64.298	80.367	96.437	112.506	120.541	128.575	136.610	144.644	152.679	160.714
2	H	1	0.0115	6.52E–03	9.65E–03	46.072	61.422	76.773	92.124	107.474	115.150	122.825	130.500	138.175	145.851	153.526
6	Li	1	7.59	3.79E+00	8.50E–03	44.167	58.883	73.600	88.316	103.032	110.390	117.748	125.106	132.464	139.822	147.180
139	La	7/2	99.910	3.56E+02	6.06E–02	42.395	56.521	70.647	84.772	98.898	105.961	113.023	120.086	127.149	134.212	141.275
9	Be	3/2	100.0	8.15E+01	1.39E–02	42.174	56.226	70.277	84.329	98.381	105.407	112.433	119.459	126.485	133.510	140.536
17	O	5/2	0.038	6.50E–02	2.91E–02	40.687	54.243	67.800	81.356	94.913	101.691	108.469	115.248	122.026	128.804	135.582
138	La	5	0.090	4.97E–01	9.40E–02	39.600	52.794	65.989	79.183	92.377	98.974	105.572	112.169	118.766	125.363	131.960
133	Cs	7/2	100.0	2.84E+02	4.84E–02	39.365	52.482	65.598	78.714	91.830	98.388	104.946	111.504	118.062	124.620	131.178
123	Sb	7/2	42.79	1.17E+02	4.66E–02	38.894	51.854	64.813	77.772	90.731	97.211	103.691	110.170	116.650	123.129	129.609
181	Ta	7/2	99.988	2.20E+02	3.74E–02	35.984	47.974	59.964	71.953	83.943	89.938	95.932	101.927	107.922	113.917	119.912
175	Lu	7/2	97.41	1.79E+02	3.13E–02	34.27	45.69	57.11	68.53	79.94	85.65	91.36	97.07	102.78	108.49	114.20
137	Ba	3/2	11.232	4.62E+00	7.00E–03	33.353	44.466	55.579	66.692	77.805	83.361	88.918	94.474	100.031	105.587	111.144
153	Eu	5/2	52.19	4.73E+01	1.54E–02	32.94	43.91	54.88	65.86	76.83	82.32	87.80	93.29	98.78	104.26	109.75
10	B	3	19.9	2.32E+01	1.99E–02	32.245	42.989	53.732	64.476	75.220	80.591	85.963	91.335	96.707	102.079	107.451
15	N	1/2	0.364	2.23E–02	1.04E–03	30.423	40.560	50.697	60.834	70.971	76.039	81.107	86.176	91.244	96.312	101.381
50	V	6	0.250	8.18E–01	5.57E–02	29.924	39.894	49.865	59.835	69.805	74.790	79.775	84.761	89.746	94.731	99.716
135	Ba	3/2	6.592	1.94E+00	5.01E–03	29.816	39.751	49.685	59.620	69.554	74.521	79.489	84.456	89.423	94.390	99.357
35	Cl	3/2	75.76	2.10E+01	4.72E–03	29.406	39.204	49.002	58.800	68.598	73.497	78.396	83.295	88.194	93.093	97.992
85	Rb	5/2	72.17	4.50E+01	1.06E–02	28.977	38.632	48.287	57.942	67.597	72.425	77.252	82.080	86.907	91.735	96.562
91	Zr	5/2	11.22	6.26E+00	9.49E–03	27.901	37.197	46.494	55.790	65.086	69.734	74.382	79.031	83.679	88.327	92.975
61	Ni	3/2	1.1399	2.40E–01	3.59E–03	26.820	35.756	44.692	53.628	62.564	67.032	71.500	75.968	80.436	84.904	89.372
169	Tm	1/2	100.0	3.32E+00	5.66E–04	24.82	33.10	41.37	49.64	57.91	62.04	66.18	70.32	74.45	78.59	82.72
131	Xe	3/2	21.2324	3.51E+00	2.82E–03	24.742	32.986	41.230	49.474	57.718	61.840	65.962	70.084	74.206	78.328	82.450
37	Cl	3/2	24.24	3.88E+00	2.72E–03	24.478	32.634	40.789	48.945	57.101	61.179	65.256	69.334	73.412	77.490	81.568
176	Lu	7	2.59	6.05E+00	3.98E–02	24.33	32.43	40.53	48.64	56.74	60.80	64.85	68.90	72.95	77.01	81.06
21	Ne	3/2	0.27	3.91E–02	2.46E–03	23.693	31.587	39.482	47.376	55.270	59.217	63.165	67.112	71.059	75.006	78.953
189	Os	3/2	16.15	2.32E+00	2.44E–03	23.306	31.072	38.837	46.602	54.368	58.251	62.133	66.016	69.899	73.781	77.664
33	S	3/2	0.75	1.00E–01	2.27E–03	23.038	30.714	38.390	46.066	53.742	57.580	61.418	65.256	69.094	72.932	76.770
14	N	1	99.636	5.90E+00	1.01E–03	21.688	28.915	36.141	43.367	50.594	54.207	57.820	61.433	65.046	68.659	72.273
43	Ca	7/2	0.135	5.10E–02	6.43E–03	20.199	26.929	33.659	40.389	47.119	50.484	53.849	57.214	60.579	63.944	67.309

NMR Frequencies vs. Bruker Field Strengths – sorted with decreasing Larmor frequency

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
				Natural rel. ^{13}C	Molar rel. ^{1}H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
97	Mo	5/2	9.56	1.96E+00	3.49E–03	19.970	26.623	33.277	39.931	46.585	49.911	53.238	56.565	59.892	63.219	66.546
201	Hg	3/2	13.18	1.16E+00	1.49E–03	19.843	26.455	33.067	39.678	46.290	49.595	52.901	56.207	59.513	62.819	66.124
95	Mo	5/2	15.90	3.06E+00	3.27E–03	19.559	26.076	32.593	39.110	45.627	48.885	52.144	55.402	58.661	61.919	65.178
67	Zn	5/2	4.102	6.92E–01	2.87E–03	18.779	25.035	31.292	37.549	43.806	46.934	50.063	53.191	56.319	59.448	62.576
25	Mg	5/2	10.00	1.58E+00	2.68E–03	18.373	24.494	30.616	36.738	42.859	45.920	48.981	52.042	55.103	58.163	61.224
53	Cr	3/2	9.501	5.07E–01	9.08E–04	16.965	22.617	28.270	33.922	39.575	42.401	45.227	48.054	50.880	53.706	56.532
49	Ti	7/2	5.41	1.20E+00	3.78E–03	16.924	22.563	28.203	33.842	39.481	42.300	45.120	47.939	50.759	53.578	56.398
47	Ti	5/2	7.44	9.18E–01	2.10E–03	16.920	22.557	28.195	33.833	39.470	42.289	45.108	47.926	50.745	53.564	56.383
143	Nd	7/2	12.2	2.43E+00	3.39E–03	16.35	21.80	27.25	32.69	38.14	40.86	43.59	46.31	49.04	51.76	54.48
101	Ru	5/2	17.06	1.58E+00	1.57E–03	15.491	20.652	25.814	30.975	36.136	38.717	41.298	43.878	46.459	49.040	51.620
89	Y	1/2	100.0	7.00E–01	1.19E–04	14.707	19.607	24.507	29.408	34.308	36.758	39.208	41.658	44.108	46.558	49.008
173	Yb	5/2	16.13	1.28E+00	1.35E–03	14.61	19.48	24.35	29.22	34.09	36.52	38.96	41.39	43.83	46.26	48.69
163	Dy	5/2	24.896	1.91E+00	1.31E–03	14.46	19.28	24.10	28.92	33.74	36.15	38.56	40.97	43.38	45.79	48.20
39	K	3/2	93.258	2.79E+00	5.10E–04	14.005	18.672	23.338	28.004	32.671	35.004	37.337	39.670	42.003	44.337	46.670
109	Ag	1/2	48.161	2.90E–01	1.02E–04	13.967	18.620	23.274	27.927	32.581	34.908	37.234	39.561	41.888	44.215	46.541
99	Ru	5/2	12.76	8.46E–01	1.13E–03	13.821	18.427	23.032	27.637	32.242	34.545	36.847	39.150	41.452	43.755	46.057
105	Pd	5/2	22.33	1.49E+00	1.13E–03	13.734	18.310	22.886	27.463	32.039	34.327	36.615	38.903	41.191	43.479	45.767
87	Sr	9/2	7.00	1.12E+00	2.72E–03	13.007	17.341	21.675	26.009	30.342	32.509	34.676	36.843	39.010	41.177	43.344
147	Sm	7/2	14.99	1.34E+00	1.52E–03	12.51	16.68	20.84	25.01	29.18	31.26	33.35	35.43	37.52	39.60	41.68
183	W	1/2	14.31	6.31E–02	7.50E–05	12.505	16.671	20.837	25.004	29.170	31.253	33.337	35.420	37.503	39.586	41.669
177	Hf	7/2	18.60	1.53E+00	1.40E–03	12.18	16.24	20.30	24.36	28.42	30.45	32.48	34.51	36.53	38.56	40.59
107	Ag	1/2	51.839	2.05E–01	6.74E–05	12.149	16.197	20.244	24.292	28.340	30.364	32.388	34.412	36.436	38.460	40.483
157	Gd	3/2	15.65	3.00E–01	3.26E–04	12.08	16.11	20.13	24.16	28.19	30.20	32.21	34.22	36.24	38.25	40.26
83	Kr	9/2	11.500	1.28E+00	1.90E–03	11.548	15.395	19.243	23.091	26.938	28.862	30.786	32.710	34.633	36.557	38.481
73	Ge	9/2	7.76	6.44E–01	1.41E–03	10.469	13.958	17.446	20.934	24.423	26.167	27.911	29.655	31.399	33.144	34.888
161	Dy	5/2	18.889	5.26E–01	4.74E–04	10.32	13.75	17.19	20.63	24.07	25.78	27.50	29.22	30.94	32.66	34.38
149	Sm	7/2	13.82	6.92E–01	8.52E–04	10.31	13.75	17.18	20.62	24.06	25.77	27.49	29.21	30.93	32.64	34.36
145	Nd	7/2	8.3	3.87E–01	7.93E–04	10.07	13.43	16.78	20.14	23.49	25.17	26.85	28.53	30.20	31.88	33.56
57	Fe	1/2	2.119	4.25E–03	3.42E–05	9.718	12.955	16.193	19.431	22.669	24.288	25.906	27.525	29.144	30.763	32.382
103	Rh	1/2	100.0	1.86E–01	3.17E–05	9.563	12.750	15.936	19.123	22.309	23.902	25.496	27.089	28.682	30.275	31.869
155	Gd	3/2	14.80	1.26E–01	1.45E–04	9.21	12.28	15.35	18.42	21.49	23.03	24.56	26.10	27.63	29.17	30.70
167	Er	7/2	22.869	6.77E–01	5.04E–04	8.66	11.54	14.42	17.31	20.19	21.63	23.08	24.52	25.96	27.40	28.85
41	K	3/2	6.730	3.34E–02	8.44E–05	7.687	10.249	12.810	15.371	17.932	19.213	20.494	21.774	23.055	24.336	25.616
179	Hf	9/2	13.62	4.38E–01	5.47E–04	7.65	10.20	12.75	15.30	17.85	19.13	20.40	21.68	22.95	24.23	25.50
187	Os	1/2	1.96	1.43E–03	1.24E–05	6.850	9.132	11.415	13.697	15.979	17.120	18.262	19.403	20.544	21.685	22.826
193	Ir	3/2	62.7	1.37E–01	3.73E–05	5.86	7.82	9.77	11.73	13.68	14.66	15.63	16.61	17.59	18.56	19.54
235	U	7/2	0.7204	6.53E–03	1.54E–04	5.527	7.368	9.209	11.051	12.892	13.813	14.734	15.654	16.575	17.496	18.416
191	Ir	3/2	37.3	6.38E–02	2.91E–05	5.40	7.20	9.00	10.79	12.59	13.49	14.39	15.29	16.19	17.09	17.99
197	Au	3/2	100.0	1.62E–01	2.76E–05	5.31	7.08	8.84	10.61	12.38	13.26	14.15	15.03	15.92	16.80	17.69

NMR Properties of Selected Isotopes

Z = proton number, **A** = mass number, **Half-Life** where appropriate in years (y), days (d), hours (h), minutes (m); ***I*** = spin quantum number; **NA** = natural abundance (IUPAC 2003); $\boldsymbol{\mu_z}$ = z-component of nuclear magnetic moment in units of the nuclear magneton (μ_N); ***Q*** = electric quadrupole moment in units of $fm^2 = 10^{-30} m^2$ (1 fm^2 = 0.01 barns); calc. magnetogyric ratio $\gamma = \mu_z/\hbar\, I$. Note: for $\boldsymbol{\mu_z}$ and ***Q*** the experimental uncertainty begins with the last significant digit.

			Isotope (half-life)	**Spin**	**Nat. Abund. 2003** (TICE 2001)	**Rel. Nucl. Magn. Mom.** (measured)	**Quadrupole Moment**	**Magnetogyric Ratio** (calc., free atom)
Z	**A**	**Sym**	**Name**	***I***	**NA** (%)	$\boldsymbol{\mu_z}$ / μ_N	***Q*** [fm^2]	γ [10^7 rad s^{-1} T^{-1}]
0	1	n	Neutron	1/2		-1.9130427		-18.3247183
1	1	H	Hydrogen	1/2	99.9885	2.79284734		26.7522208
	2	H (D)	Deuterium	1	0.0115	0.857438228	0.286	4.10662919
	3	H (T)	Tritium (12.32 y)	1/2		2.97896244		28.5349865
2	3	He	Helium	1/2	0.000134	-2.12749772		-20.3789473
3	6	Li	Lithium	1	7.59	0.8220473	-0.0808	3.937127
	7	Li	Lithium	3/2	92.41	3.2564625	-4.01	10.397704
4	9	Be	Beryllium	3/2	100	-1.17749	5.288	-3.75966
5	10	B	Boron	3	19.9	1.80064478	8.459	2.87467955
	11	B	Boron	3/2	80.1	2.688649	4.059	8.584707
6	13	C	Carbon	1/2	1.07	0.702412		6.728286
7	14	N	Nitrogen	1	99.636	0.40376100	2.044	1.9337798
	15	N	Nitrogen	1/2	0.364	-0.28318884		-2.7126189
8	17	O	Oxygen	5/2	0.038	-1.89379	-2.558	-3.62806
9	19	F	Fluorine	1/2	100	2.626868		25.16233
10	21	Ne	Neon	3/2	0.27	-0.661797	10.155	-2.113081
11	23	Na	Sodium (Natrium)	3/2	100	2.2176556	10.4	7.0808516
12	25	Mg	Magnesium	5/2	10.00	-0.85545	19.94	-1.63884
13	26	Al	Alumin(i)um (7.17E5 y)	5		2.804	27	2.686
13	27	Al	Alumin(i)um	5/2	100	3.6415069	14.66	6.9762780
14	29	Si	Silicon	1/2	4.685	-0.55529		-5.31903
15	31	P	Phosphorus	1/2	100	1.13160		10.8394
16	33	S	Sulfur	3/2	0.75	0.643821	-6.78	2.055685
17	35	Cl	Chlorine	3/2	75.76	0.8218743	-8.165	2.6241991
	37	Cl	Chlorine	3/2	24.24	0.6841236	-6.435	2.1843688
18	39	Ar	Argon (269 y)	7/2		-1.59		-2.17
19	39	K	Potassium (Kalium)	3/2	93.258	0.3915073	5.85	1.2500612
	40	K	Potassium (1.248E9 y)	4	0.0117	-1.298100	-7.3	-1.554286
	41	K	Potassium	3/2	6.730	0.21489274	7.11	0.68614062
20	41	Ca	Calcium (1.02E5 y)	7/2		-1.594781	-6.7	-2.182306
	43	Ca	Calcium	7/2	0.135	-1.317643	-4.08	-1.803069
21	45	Sc	Scandium	7/2	100	4.756487	-22.0	6.508800
22	47	Ti	Titanium	5/2	7.44	-0.78848	30.2	-1.51054
	49	Ti	Titanium	7/2	5.41	-1.10417	24.7	-1.51095
23	50	V	Vanadium (1.4E17 y)	6	0.250	3.345689	21	2.670650
	51	V	Vanadium	7/2	99.750	5.1487057	-5.2	7.0455139
24	53	Cr	Chromium	3/2	9.501	-0.47454	-15	-1.51518
25	53	Mn	Manganese (3.74E6 y)	7/2		*5.024*		6.875
	55	Mn	Manganese	5/2	100	3.46871790	33	6.64525453
26	57	Fe	Iron, Ferrum	1/2	2.119	0.09062300		0.8680627
	59	Fe	Iron (44.507 d)	3/2		-0.3358		-1.0722
27	59	Co	Cobalt	7/2	100	4.627	42 s	6.332
	60	Co	Cobalt (1925.2 d)	5		3.799	44	3.639
28	61	Ni	Nickel	3/2	1.1399	-0.75002	16.2	-2.39477
29	63	Cu	Copper, Cuprum	3/2	69.15	2.227346	-22.0	7.111791
	65	Cu	Copper, Cuprum	3/2	30.85	2.3816	-20.4	7.6043
30	67	Zn	Zinc	5/2	4.102	0.8752049	15.0	1.6766885
31	69	Ga	Gallium	3/2	60.108	2.01659	17.1	6.43886
	71	Ga	Gallium	3/2	39.892	2.56227	10.7	8.18117
32	73	Ge	Germanium	9/2	7.76	-0.8794677	-19.6	-0.9360306
33	75	As	Arsenic	3/2	100	1.43947	31.4	4.59615
34	77	Se	Selenium	1/2	7.63	0.5350743		5.125388

NMR Properties of Selected Isotopes

Theor. NMR freq. ν_o calc. from γ and scaled to ^{1}H = 100.0 MHz; Molar Receptivity **R_M(H)** relative to equal number of protons is proportional to $\gamma^3 I(I+1)$; Receptivity at nat. abundance **R_{NA}(C)** relative to ^{13}C; recommended Reference sample (IUPAC 2001); *experimental* reson. freq. of ref. sample on the unified Ξ scale (at B_0 where TMS (^{1}H) = 100.0 MHz).
Numbers containing E are in exponential format.

		Theoretical NMR Freq. (free atom)	**Molar Receptivity** (rel. ^{1}H)	**Receptivity at Nat. Abund.** (rel. ^{13}C)	**Reference Sample**	**Measured. NMR Freq.** (rel. ^{1}H ref.)
A	**Sym**	ν_o [MHz]	**R_M(H)**	**R_{NA}(C)**	**Reference**	Ξ [MHz]
1	n	68.4979	3.21E–01			
1	H	100.0000	**1.00E+00**	5.87E+03	1% Me_4Si in $CDCl_3$	100.000000
2	D	15.3506	9.65E–03	6.52E–03	$(CD_3)_4Si$ neat	15.350609
3	T	106.6640	1.21E+00		TMS-T_1	106.663974
3	He	76.1767	4.42E–01	3.48E–03	He gas	76.178976
6	Li	14.7170	8.50E–03	3.79E+00	9.7 m LiCl in D_2O	14.716086
7	Li	38.8667	2.94E–01	1.59E+03	9.7 m LiCl in D_2O	38.863797
9	Be	14.0536	1.39E–02	8.15E+01	0.43 m $BeSO_4$ in D_2O	14.051813
10	B	10.7456	1.99E–02	2.32E+01	15% $BF_3.Et_2O$ in $CDCl_3$	10.743658
11	B	32.0897	1.65E–01	7.77E+02	15% $BF_3.Et_2O$ in $CDCl_3$	32.083974
13	C	25.1504	1.59E–02	**1.00E+00**	1% Me_4Si in $CDCl_3$ DSS in D_2O	25.145020 25.144953
14	N	7.2285	1.01E–03	5.90E+00	$MeNO_2$ + 10% $CDCl_3$	7.226317
15	N	10.1398	1.04E–03	2.23E–02	$MeNO_2$ + 10% $CDCl_3$ liquid NH_3	10.136767 10.132767
17	O	13.5617	2.91E–02	6.50E–02	D_2O	13.556457
19	F	94.0570	8.32E–01	4.89E+03	CCl_3F	94.094011
21	Ne	7.8987	2.46E–03	3.91E–02	Neon gas, 1.1 MPa	7.894296
23	Na	26.4683	9.27E–02	5.45E+02	0.1 M NaCl in D_2O	26.451900
25	Mg	6.1260	2.68E–03	1.58E+00	11 M $MgCl_2$ in D_2O	6.121635
26	Al	10.0399	4.05E–02			
27	Al	26.0774	2.07E–01	1.22E+03	1.1 m $Al(NO_3)_3$ in D_2O	26.056859
29	Si	19.8826	7.86E–03	2.16E+00	1% Me_4Si in $CDCl_3$	19.867187
31	P	40.5178	6.65E–02	3.91E+02	H_3PO_4 external $(MeO)_3PO$ internal	40.480742 40.480864
33	S	7.6842	2.27E–03	1.00E–01	$(NH_4)_2SO_4$ in D_2O (sat.)	7.676000
35	Cl	9.8093	4.72E–03	2.10E+01	0.1 M NaCl in D_2O	9.797909
37	Cl	8.1652	2.72E–03	3.88E+00	0.1 M NaCl in D_2O	8.155725
39	Ar	8.1228	1.13E–02			
39	K	4.6727	5.10E–04	2.79E+00	0.1 M KCl in D_2O	4.666373
40	K	5.8099	5.23E–03	3.59E–03	0.1 M KCl in D_2O	5.802018
41	K	2.5648	8.44E–05	3.34E–02	0.1 M KCl in D_2O	2.561305
41	Ca	8.1575	1.14E–02			
43	Ca	6.7399	6.43E–03	5.10E–02	0.1 M $CaCl_2$ in D_2O	6.730029
45	Sc	24.3299	3.02E–01	1.78E+03	0.06 M $Sc(NO_3)_3$ in D_2O	24.291747
47	Ti	5.6464	2.10E–03	9.18E–01	$TiCl_4$ neat + 10% C_6D_{12}	5.637534
49	Ti	5.6479	3.78E–03	1.20E+00	$TiCl_4$ neat + 10% C_6D_{12}	5.639037
50	V	9.9829	5.57E–02	8.18E–01	$VOCl_3$ + 5% C_6D_6	9.970309
51	V	26.3362	3.84E–01	2.25E+03	$VOCl_3$ + 5% C_6D_6	26.302948
53	Cr	5.6638	9.08E–04	5.07E–01	K_2CrO_4 in D_2O (sat.)	5.652496
53	Mn	25.6983	3.56E–01			
55	Mn	24.8400	1.79E–01	1.05E+03	0.82 m $KMnO_4$ in D_2O	24.789218
57	Fe	3.2448	3.42E–05	4.25E–03	$Fe(CO)_5$ + 20% C_6D_6	3.237778
59	Fe	4.0079	3.22E–04			
59	Co	23.6676	2.78E–01	1.64E+03	0.56 m $K_3[Co(CN)_6]$ in D_2O	23.727074
60	Co	13.6026	1.01E–01			
61	Ni	8.9517	3.59E–03	2.40E–01	$Ni(CO)_4$ + 5% C_6D_6	8.936051
63	Cu	26.5839	9.39E–02	3.82E+02	$[Cu(CH_3CN)_4][ClO_4]$ in CH_3CN (sat.) + 5% C_6D_6	26.515473
65	Cu	28.4250	1.15E–01	2.08E+02	$[Cu(CH_3CN)_4][ClO_4]$ in CH_3CN (sat.) + 5% C_6D_6	28.403693
67	Zn	6.2675	2.87E–03	6.92E–01	$Zn(NO_3)_3$ in D_2O (sat.)	6.256803
69	Ga	24.0685	6.97E–02	2.46E+02	1.1 m $Ga(NO_3)_3$ in D_2O	24.001354
71	Ga	30.5813	1.43E–01	3.35E+02	1.1 m $Ga(NO_3)_3$ in D_2O	30.496704
73	Ge	3.4989	1.41E–03	6.44E–01	Me_4Ge + 5% C_6D_6	3.488315
75	As	17.1804	2.54E–02	1.49E+02	0.5 M $NaAsF_6$ in CD_3CN	17.122614
77	Se	19.1587	7.03E–03	3.15E+00	Me_2Se + 5% C_6D_6	19.071513

NMR Properties of Selected Isotopes

Z	A	Sym	Name	*I*	NA (%)	μ_z / μ_N	*Q* [fm^2]	γ [10^7 rad s^{-1} T^{-1}]
	79	Se	Selenium (2.95E5 y)	7/2		-1.018	80	-1.393
35	79	Br	Bromine	3/2	50.69	2.106400	30.5	6.725619
	81	Br	Bromine	3/2	49.31	2.270562	25.4	7.249779
36	83	Kr	Krypton	9/2	11.500	-0.970669	25.9	-1.033097
37	85	Rb	Rubidium	5/2	72.17	1.3533515	27.6	2.5927059
	87	Rb	Rubidium (4.81E10 y)	3/2	27.83	2.751818	13.35	8.786403
38	87	Sr	Strontium	9/2	7.00	-1.093603	33.5	-1.163938
39	89	Y	Yttrium	1/2	100	-0.1374154		-1.316279
40	91	Zr	Zirconium	5/2	11.22	-1.30362	-17.6	-2.49743
41	93	Nb	Niobium	9/2	100	6.1705	-32	6.5674
42	95	Mo	Molybdenum	5/2	15.9	-0.9142	-2.2	-1.7514
	97	Mo	Molybdenum	5/2	9.56	-0.9335	25.5	-1.7884
	99	Mo	Molybdenum (65.924 h)	1/2		*0.375*		3.59
43	99	Tc	Technetium (2.1E5 y)	9/2		5.6847	-12.9	6.0503
44	99	Ru	Ruthenium	5/2	12.76	-0.641	7.9	-1.228
	101	Ru	Ruthenium	5/2	17.06	-0.716	45.7	-1.372
45	103	Rh	Rhodium	1/2	100	-0.08840		-0.84677
46	105	Pd	Palladium	5/2	22.33	-0.642	66	-1.230
47	107	Ag	Silver, Argentum	1/2	51.839	-0.1136797		-1.088918
	109	Ag	Silver	1/2	48.161	-0.13069		-1.2519
48	111	Cd	Cadmium	1/2	12.80	-0.5948861		-5.698315
	113	Cd	Cadmium (7.7E15 y)	1/2	12.22	-0.6223009		-5.960917
49	113	In	Indium	9/2	4.29	5.5289	79.9	5.8845
	115	In	Indium (4.41E14 y)	9/2	95.71	5.5408	81	5.8972
50	115	Sn	Tin	1/2	0.34	-0.91883		-8.8013
	117	Sn	Tin	1/2	7.68	-1.00104		-9.58880
	119	Sn	Tin (Stannum)	1/2	8.59	-1.04728		-10.0317
51	121	Sb	Antimony (Stibium)	5/2	57.21	3.3634	-36	6.4435
	123	Sb	Antimony	7/2	42.79	2.5498	-49	3.4892
	125	Sb	Antimony (2.7586 y)	7/2		*2.63*		3.60
52	123	Te	Tellurium (9.2E16 y)	1/2	0.89	-0.7369478		-7.059101
	125	Te	Tellurium	1/2	7.07	-0.8885051		-8.510843
53	127	I	Iodine	5/2	100	2.81327	-71	5.38957
	129	I	Iodine (1.57E7 y)	7/2		2.6210	-48	3.5866
54	129	Xe	Xenon	1/2	26.4006	-0.777976		-7.45210
	131	Xe	Xenon	3/2	21.2324	0.691862	-11.4	2.209077
55	133	Cs	C(a)esium	7/2	100	2.582025	-0.343	3.533256
56	135	Ba	Barium	3/2	6.592	0.838627	16.0	2.677690
	137	Ba	Barium	3/2	11.232	0.93734	24.5	2.99287
57	137	La	Lanthanum (6E4 y)	7/2		2.695	26	3.688
57	138	La	Lanthanum (1.05E11 y)	5	0.090	3.713646	45	3.557240
	139	La	Lanthanum	7/2	99.910	2.7830455	20	3.808333
58	139	Ce	Cerium (137.64 d)	3/2		*1.06*		3.38
	141	Ce	Cerium (32.508 d)	7/2		*1.09*		1.49
59	141	Pr	Praeseodymium	5/2	100	4.2754	-5.89	8.1907
60	143	Nd	Neodymium	7/2	12.2	-1.065	-63	-1.4574
	145	Nd	Neodymium	7/2	8.3	-0.656	-33	-0.898
61	145	Pm	Promethium (17.7 y)	5/2		3.8	21	7.3
62	147	Sm	Samarium (1.06E11 y)	7/2	14.99	-0.8148	-25.9	-1.115
	149	Sm	Samarium	7/2	13.82	-0.6717	7.5	-0.9192
63	151	Eu	Europium	5/2	47.81	3.4717	90.3	6.6510
	153	Eu	Europium	5/2	52.19	1.5324	241	2.9357
64	155	Gd	Gadolinium	3/2	14.80	-0.2572	127	-0.8212
	157	Gd	Gadolinium	3/2	15.65	-0.3373	135	-1.0770
65	159	Tb	Terbium	3/2	100	2.014	143.2	6.431
66	161	Dy	Dysprosium	5/2	18.889	-0.480	251	-0.920
	163	Dy	Dysprosium	5/2	24.896	0.673	265	1.289
67	163	Ho	Holmium (4570 y)	7/2		4.23	360	5.79
	165	Ho	Holmium	7/2	100	4.132	358	5.654
	166	Ho	Holmium (1200 y)	7		*3.60*	-340	2.46
68	167	Er	Erbium	7/2	22.869	-0.5639	357	-0.7716
	169	Er	Erbium (9.40 d)	1/2		0.4850		4.646
69	169	Tm	Thulium	1/2	100	-0.231		-2.21
	171	Tm	Thulium (1.92 y)	1/2		-0.228		-2.18
70	171	Yb	Ytterbium	1/2	14.28	0.49367		4.7288
	173	Yb	Ytterbium	5/2	16.13	-0.67989	280	-1.30251
71	175	Lu	Lutetium	7/2	97.41	2.232	349	3.0547

NMR Properties of Selected Isotopes

A	Sym	ν_o [MHz]	$R_M(H)$	$R_{NA}(C)$	Reference	Ξ [MHz]
79	Se	5.2072	2.97E–03			
79	Br	25.1404	7.94E–02	2.37E+02	0.01 M NaBr in D_2O	25.053980
81	Br	27.0997	9.95E–02	2.88E+02	0.01 M NaBr in D_2O	27.006518
83	Kr	3.8617	1.90E–03	1.28E+00	Kr gas	3.847600
85	Rb	9.6916	1.06E–02	4.50E+01	0.01 M RbCl in D_2O	9.654943
87	Rb	32.8436	1.77E–01	2.90E+02	0.01 M RbCl in D_2O	32.720454
87	Sr	4.3508	2.72E–03	1.12E+00	0.5 M $SrCl_2$ in D_2O	4.333822
89	Y	4.9203	1.19E–04	7.00E–01	$Y(NO_3)_3$ in H_2O/D_2O	4.900198
91	Zr	9.3354	9.49E–03	6.26E+00	$Zr(C_5H_5)_2Cl_2$ in CH_2Cl_2 (sat.) + 5% C_6D_6	9.296298
93	Nb	24.5488	4.88E–01	2.87E+03	$K[NbCl_6]$ in CH_3CN / CD_3CN (sat.)	24.476170
95	Mo	6.5467	3.27E–03	3.06E+00	2 M Na_2MoO_4 in D_2O	6.516926
97	Mo	6.6849	3.49E–03	1.96E+00	2 M Na_2MoO_4 in D_2O	6.653695
99	Mo	13.4272	2.42E–03			
99	Tc	22.6161	3.82E–01		NH_4TcO_4 in H_2O / D_2O	22.508326
99	Ru	4.5903	1.13E–03	8.46E–01	0.3 M $K_4[Ru(CN)_6]$ in D_2O	4.605151
101	Ru	5.1274	1.57E–03	1.58E+00	0.3 M $K_4[Ru(CN)_6]$ in D_2O	5.161369
103	Rh	3.1652	3.17E–05	1.86E–01	$Rh(acac)_3$ in $CDCl_3$ (sat.)	3.186447
105	Pd	4.5975	1.13E–03	1.49E+00	K_2PdCl_6 in D_2O (sat.)	4.576100
107	Ag	4.0704	6.74E–05	2.05E–01	$AgNO_3$ in D_2O (sat.)	4.047819
109	Ag	4.6795	1.02E–04	2.90E–01	$AgNO_3$ in D_2O (sat.)	4.653533
111	Cd	21.3003	9.66E–03	7.27E+00	Me_2Cd neat liq.	21.215480
113	Cd	22.2820	1.11E–02	7.94E+00	Me_2Cd neat liq.	22.193175
113	In	21.9963	3.51E–01	8.85E+01	0.1 M $In(NO_3)_3$ in D_2O + 0.5 M DNO_3	21.865755
115	In	22.0436	3.53E–01	1.99E+03	0.1 M $In(NO_3)_3$ in D_2O + 0.5 M DNO_3	21.912629
115	Sn	32.8994	3.56E–02	7.11E–01	Me_4Sn + 5% C_6D_6	32.718749
117	Sn	35.8430	4.60E–02	2.08E+01	Me_4Sn + 5% C_6D_6	35.632259
119	Sn	37.4986	5.27E–02	2.66E+01	Me_4Sn + 5% C_6D_6	37.290632
121	Sb	24.0858	1.63E–01	5.48E+02	$KSbCl_6$ in CH_3CN / CD_3CN (sat.)	23.930577
123	Sb	13.0425	4.66E–02	1.17E+02	$KSbCl_6$ in CH_3CN / CD_3CN (sat.)	12.959217
125	Sb	13.4527	5.11E–02			
123	Te	26.3870	1.84E–02	9.61E–01	Me_2Te + 5% C_6D_6	26.169742
125	Te	31.8136	3.22E–02	1.34E+01	Me_2Te + 5% C_6D_6	31.549769
127	I	20.1462	9.54E–02	5.60E+02	0.01 M KI in D_2O	20.007486
129	I	13.4067	5.06E–02			
129	Xe	27.8560	2.16E–02	3.35E+01	$XeOF_4$ neat liq.	27.810186
131	Xe	8.2575	2.82E–03	3.51E+00	$XeOF_4$ neat liq.	8.243921
133	Cs	13.2073	4.84E–02	2.84E+02	0.1 M $CsNO_3$ in D_2O	13.116142
135	Ba	10.0092	5.01E–03	1.94E+00	0.5 M $BaCl_2$ in D_2O	9.934457
137	Ba	11.1874	7.00E–03	4.62E+00	0.5 M $BaCl_2$ in D_2O	11.112928
137	La	13.7852	5.50E–02			
138	La	13.2970	9.40E–02	4.97E–01	$LaCl_3$ in D_2O / H_2O	13.194300
139	La	14.2356	6.06E–02	3.56E+02	0.01 M $LaCl_3$ in D_2O	14.125641
139	Ce	12.6514	1.01E–02			
141	Ce	5.5755	3.64E–03			
141	Pr	30.6168	3.35E–01	1.97E+03		
143	Nd	5.4476	3.39E–03	2.43E+00		
145	Nd	3.3555	7.93E–04	3.87E–01		
145	Pm	27.2124	2.35E–01			
147	Sm	4.1678	1.52E–03	1.34E+00		
149	Sm	3.4358	8.52E–04	6.92E–01		
151	Eu	24.8614	1.79E–01	5.04E+02		
153	Eu	10.9737	1.54E–02	4.73E+01		
155	Gd	3.0697	1.45E–04	1.26E–01		
157	Gd	4.0258	3.26E–04	3.00E–01		
159	Tb	24.0376	6.94E–02	4.08E+02		
161	Dy	3.4374	4.74E–04	5.26E–01		
163	Dy	4.8195	1.31E–03	1.91E+00		
163	Ho	21.6369	2.13E–01			
165	Ho	21.1356	1.98E–01	1.16E+03		
166	Ho	9.2072	5.83E–02		(+6 keV excited state)	
167	Er	2.8842	5.04E–04	6.77E–01		
169	Er	17.3658	5.24E–03			
169	Tm	8.2711	5.66E–04	3.32E+00		
171	Tm	8.1637	5.44E–04			
171	Yb	17.6762	5.52E–03	4.63E+00	0.171 M $Yb(\eta\text{-}C_5Me_5)_2(THF)_2$ in THF	17.499306
173	Yb	4.8688	1.35E–03	1.28E+00		
175	Lu	11.4185	3.13E–02	1.79E+02		

NMR Properties of Selected Isotopes

Z	A	Sym	Name	*I*	NA (%)	μ_z / μ_N	*Q* [fm^2]	γ [10^7 rad s^{-1} T^{-1}]
	176	Lu	Lutetium (3.78E10 y)	7	2.59	3.169	497	2.168
72	177	Hf	Hafnium	7/2	18.60	0.7935	337	1.0858
	179	Hf	Hafnium	9/2	13.62	-0.641	379	-0.682
73	179	Ta	Tantalum (1.82 y)	7/2		2.289	337	3.132
	180	Ta	Tantalum (1.2E15 y)	9	0.012	4.825	495	2.568
	181	Ta	Tantalum	7/2	99.988	2.3705	317	3.2438
74	183	W	Tungsten (Wolfram)	1/2	14.31	0.11778476		1.1282407
75	185	Re	Rhenium	5/2	37.40	3.1871	218	6.1057
	187	Re	Rhenium (4.35E10 y)	5/2	62.60	3.2197	207	6.1682
76	187	Os	Osmium	1/2	1.96	0.06465189		0.6192897
	189	Os	Osmium	3/2	16.15	0.659933	85.6	2.107130
77	191	Ir	Iridium	3/2	37.3	0.1507	81.6	0.4812
	193	Ir	Iridium	3/2	62.7	0.1637	75.1	0.5227
78	195	Pt	Platinum	1/2	33.832	0.60952		5.8385
79	197	Au	Gold, Aurum	3/2	100	0.148158	54.7	0.473060
80	199	Hg	Mercury, Hydrargyrum	1/2	16.87	0.5058855		4.845793
	201	Hg	Mercury	3/2	13.18	-0.560226	38.6	-1.788770
81	203	Tl	Thallium	1/2	29.52	1.6222579		15.539339
	205	Tl	Thallium	1/2	70.48	1.6382146		15.692186
82	205	Pb	Lead (1.73E7 y)	5/2		0.7117	23	1.3635
	207	Pb	Lead (Plumbum)	1/2	22.1	0.58219		5.5767
83	209	Bi	Bismuth	9/2	100	4.1103	-51.6	4.3747
84	209	Po	Polonium (102 y)	1/2		0.68		6.51
86	211	Rn	Radon (14.6 h)	1/2		0.601		5.76
87	212	Fr	Francium (19.3 m)	5		4.62	-10	4.43
88	225	Ra	Radium (14.9 d)	1/2		-0.734		-7.03
89	227	Ac	Actinium (21.77 y)	3/2		1.1	170	3.5
90	229	Th	Thorium (7.34E3 y)	5/2		0.46	430	0.88
91	231	Pa	Protactinium (3.25E4 y)	3/2	100	*2.01*	-172	6.42
92	233	U	Uranium (1.592E5 y)	5/2		*0.59*	366.3	1.13
	235	U	Uranium (7.04E8 y)	7/2	0.7204	-0.38	493.6	-0.52
	238	U	Uranium (4.468E9 y)	0	99.274		1390	
93	237	Np	Neptunium (2.14E6 y)	5/2		3.14	386.6	6.02
94	239	Pu	Plutonium (2.410E4 y)	1/2		0.203		1.94
	241	Pu	Plutonium (14.4 y)	5/2		-0.68	560	-1.30
95	241	Am	Americium (432.7 y)	5/2		1.58	314	3.03
	243	Am	Americium (7.37E3 y)	5/2		1.50	286	2.87
96	243	Cm	Curium (29.1 y)	5/2		*0.41*		0.79
	245	Cm	Curium (8.48E3 y)	7/2		*0.5*		0.68
	247	Cm	Curium (1.56E7 y)	9/2		*0.37*		0.39
97	247	Bk	Berkelium (1.4E2 y)	(3/2)		*no data*		
	249	Bk	Berkelium (320 d)	7/2		*2.0*		2.7
98	251	Cf	Californium (9.0E2 y)	1/2		*no data*		
99	252	Es	Einsteinium (472 d)	(5)		*no data*		
	253	Es	Einsteinium (20.47 d)	7/2		4.10	670	5.61
100	253	Fm	Fermium (3.0 d)	(1/2)		*no data*		
	257	Fm	Fermium (100.5 d)	(9/2)		*no data*		

This Table (updated Oct. 2009) was assembled and calculated by W.E. Hull using information from the following sources:

De Laeter et al. *Pure Appl Chem* 75 (2003) 683-800. (isotope abundances)

Harris RK, et al. *Pure Appl Chem* 73 (2001) 1795-1818 and 80 (2008) 59-84. (shift references)

Mills I, et al. *Quantities, Units and Symbols in Physical Chemistry* (IUPAC recommendations 1993, corrections 1995). Blackwell Scientific (1993, 1995).

Pyykkö P. Spectroscopic nuclear quadrupole moments. Mol. Phys. 99 (2001) 1617-1629.

NMR Properties of Selected Isotopes

A	Sym	ν_o [MHz]	$R_M(H)$	$R_{NA}(C)$	Reference	Ξ [MHz]
176	Lu	8.1049	3.98E–02	6.05E+00		
177	Hf	4.0588	1.40E–03	1.53E+00		
179	Hf	2.5502	5.47E–04	4.38E–01		
179	Ta	11.7085	3.37E–02			
180	Ta	9.5979	1.06E–01	7.48E–02	(+77 keV excited state)	
181	Ta	12.1254	3.74E–02	2.20E+02	$KTaCl_6$ in CH_3CN (sat.)	11.989600
183	W	4.2174	7.50E–05	6.31E–02	1 M Na_2WO_4 in D_2O	4.166387
185	Re	22.8233	1.39E–01	3.05E+02	0.1 M $KReO_4$ in D_2O	22.524600
187	Re	23.0568	1.43E–01	5.26E+02	0.1 M $KReO_4$ in D_2O	22.751600
187	Os	2.3149	1.24E–05	1.43E–03	0.98 M OsO_4 in CCl_4	2.282331
189	Os	7.8765	2.44E–03	2.32E+00	0.98 M OsO_4 in CCl_4	7.765400
191	Ir	1.7986	2.91E–05	6.38E–02		
193	Ir	1.9538	3.73E–05	1.37E–01		
195	Pt	21.8243	1.04E–02	2.07E+01	1.2 M Na_2PtCl_6 in D_2O	21.496784
197	Au	1.7683	2.76E–05	1.62E–01		
199	Hg	18.1136	5.94E–03	5.89E+00	Me_2Hg neat liq. (toxic!)	17.910822
201	Hg	6.6864	1.49E–03	1.16E+00	Me_2Hg neat liq. (toxic!)	6.611583
203	Tl	58.0862	1.96E–01	3.40E+02	$Tl(NO_3)_3$	57.123200
205	Tl	58.6575	2.02E–01	8.36E+02	$Tl(NO_3)_3$	57.683838
205	Pb	5.0966	1.54E–03			
207	Pb	20.8458	9.06E–03	1.18E+01	Me_4Pb + 5% C_6D_6	20.920599
209	Bi	16.3525	1.44E–01	8.48E+02	$Bi(NO_3)_2$ sat. in conc. HNO_3 + 50% D_2O	16.069288
209	Po	24.3479	1.44E–02			
211	Rn	21.5193	9.97E–03			
212	Fr	16.5423	1.81E–01			
225	Ra	26.2814	1.82E–02			
227	Ac	13.1288	1.13E–02			
229	Th	3.2941	4.17E–04			
231	Pa	23.9899	6.90E–02	4.06E+02		
233	U	4.2251	8.80E–04			
235	U	1.9437	1.54E–04	6.53E–03	UF_6 + 10% C_6D_6	1.841400
238	U					
237	Np	22.4860	1.33E–01			
239	Pu	7.2686	3.84E–04			
241	Pu	4.8696	1.35E–03			
241	Am	11.3146	1.69E–02			
243	Am	10.7417	1.45E–02			
243	Cm	2.9361	2.95E–04			
245	Cm	2.5576	3.51E–04			
247	Cm	1.4720	1.05E–04			
249	Bk	10.2302	2.25E–02			
253	Es	20.9719	1.94E–01			

Stone NJ. *Table of Nuclear Magnetic Dipole and Electric Quadrupole Moments (2001)* [http://www.nndc.bnl.gov/nndc/stone_moments/nuclear-moments.pdf].
LBNL Isotopes Project Nuclear Data Dissemination Home Page. *Table of Nuclear Moments* [http://ie.lbl.gov/toipdf/mometbl.pdf].
NUDAT 2 half-life data: http://www.nndc.bnl.gov/

NMR Tables

Isotopes sorted according to spin and nucleon numbers

Isotope			Spin	Isotope			Spin	Isotope			Spin
1	H	Hydrogen	1/2	39	K	Potassium	3/2	173	Yb	Ytterbium	5/2
3	H	Tritium *	1/2	41	K	Potassium	3/2	185	Re	Rhenium	5/2
3	He	Helium	1/2	53	Cr	Chromium	3/2	187	Re	Rhenium	5/2
13	C	Carbon	1/2	61	Ni	Nickel	3/2	229	Th	Thorium *	5/2
15	N	Nitrogen	1/2	63	Cu	Copper	3/2	237	Np	Neptunium *	5/2
19	F	Fluorine	1/2	65	Cu	Copper	3/2	241	Am	Americium *	5/2
29	Si	Silicon	1/2	69	Ga	Gallium	3/2	243	Am	Americium *	5/2
31	P	Phosphorus	1/2	71	Ga	Gallium	3/2	10	B	Boron	3
57	Fe	Iron	1/2	75	As	Arsenic	3/2	39	Ar	Argon *	7/2
77	Se	Selenium	1/2	79	Br	Bromine	3/2	43	Ca	Calcium	7/2
89	Y	Yttrium	1/2	81	Br	Bromine	3/2	45	Sc	Scandium	7/2
103	Rh	Rhodium	1/2	87	Rb	Rubidium	3/2	49	Ti	Titanium	7/2
107	Ag	Silver	1/2	131	Xe	Xenon	3/2	51	V	Vanadium	7/2
109	Ag	Silver	1/2	135	Ba	Barium	3/2	59	Co	Cobalt	7/2
111	Cd	Cadmium	1/2	137	Ba	Barium	3/2	123	Sb	Antimony	7/2
113	Cd	Cadmium	1/2	139	Ce	Cerium *	3/2	133	Cs	C(a)esium	7/2
115	Sn	Tin	1/2	155	Gd	Gadolinium	3/2	139	La	Lanthanum	7/2
117	Sn	Tin	1/2	157	Gd	Gadolinium	3/2	143	Nd	Neodymium	7/2
119	Sn	Tin	1/2	159	Tb	Terbium	3/2	145	Nd	Neodymium	7/2
123	Te	Tellurium	1/2	189	Os	Osmium	3/2	147	Sm	Samarium	7/2
125	Te	Tellurium	1/2	191	Ir	Iridium	3/2	149	Sm	Samarium	7/2
129	Xe	Xenon	1/2	193	Ir	Iridium	3/2	165	Ho	Holmium	7/2
169	Tm	Thulium	1/2	197	Au	Gold	3/2	167	Er	Erbium	7/2
171	Yb	Ytterbium	1/2	201	Hg	Mercury	3/2	175	Lu	Lutetium	7/2
183	W	Tungsten	1/2	227	Ac	Actinium *	3/2	177	Hf	Hafnium	7/2
187	Os	Osmium	1/2	231	Pa	Protactinium *	3/2	181	Ta	Tantalum	7/2
195	Pt	Platinum	1/2	17	O	Oxygen	5/2	235	U	Uranium *	7/2
199	Hg	Mercury	1/2	25	Mg	Magnesium	5/2	245	Cm	Curium *	7/2
203	Tl	Thallium	1/2	27	Al	Alumin(i)um	5/2	249	Bk	Berkelium *	7/2
205	Tl	Thallium	1/2	47	Ti	Titanium	5/2	253	Es	Einsteinium *	7/2
207	Pb	Lead	1/2	55	Mn	Manganese	5/2	73	Ge	Germanium	9/2
209	Po	Polonium *	1/2	67	Zn	Zinc	5/2	83	Kr	Krypton	9/2
211	Rn	Radon *	1/2	85	Rb	Rubidium	5/2	87	Sr	Strontium	9/2
225	Ra	Radium *	1/2	91	Zr	Zirconium	5/2	93	Nb	Niobium	9/2
239	Pu	Plutonium *	1/2	95	Mo	Molybdenum	5/2	99	Tc	Technetium *	9/2
251	Cf	Californium *	1/2	97	Mo	Molybdenum	5/2	113	In	Indium	9/2
2	H	Deuterium	1	99	Ru	Ruthenium	5/2	115	In	Indium	9/2
6	Li	Lithium	1	101	Ru	Ruthenium	5/2	179	Hf	Hafnium	9/2
14	N	Nitrogen	1	105	Pd	Palladium	5/2	209	Bi	Bismuth	9/2
7	Li	Lithium	3/2	121	Sb	Antimony	5/2	138	La	Lanthanum	5
9	Be	Beryllium	3/2	127	I	Iodine	5/2	212	Fr	Francium *	5
11	B	Boron	3/2	141	Pr	Praeseodymium	5/2	50	V	Vanadium	6
21	Ne	Neon	3/2	145	Pm	Promethium *	5/2	176	Lu	Lutetium	7
23	Na	Sodium	3/2	151	Eu	Europium	5/2				
33	S	Sulfur	3/2	153	Eu	Europium	5/2				
35	Cl	Chlorine	3/2	161	Dy	Dysprosium	5/2				
37	Cl	Chlorine	3/2	163	Dy	Dysprosium	5/2				

* Unstable isotope with lifetime suitable for NMR.

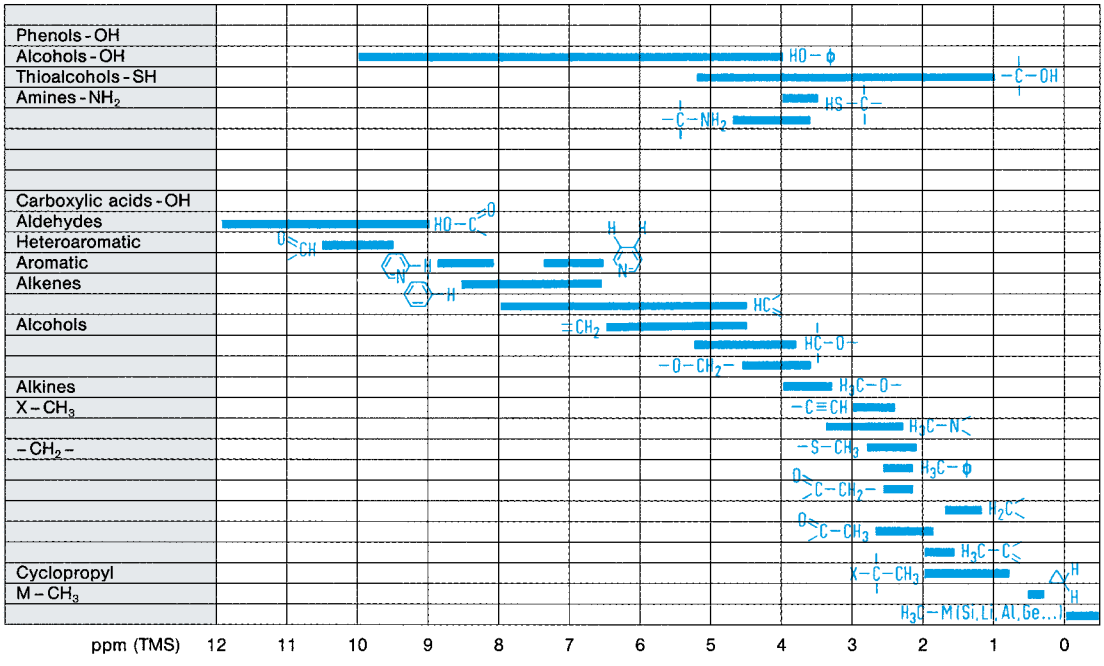
Properties of Selected Deuterated Solvents for NMR

Solvent	Formula	MW_{ave}	Density $[d_4^{20}]$	MP [°C]	BP [°C]	RI $[n_D^{20}]$	Dielec. [ε]	^{1}H shift (Mult.) [ppm]	J(HD) [Hz]	^{13}C Shift (Mult.) [ppm]	J(CD) [Hz]	H_2O/HDO Shift [ppm]
Acetic Acid-d4	$C_2D_4O_2$	64.08	1.119	15.9	115.5	1.368	6.1	11.65 2.04 (5)	2.2	178.99 20 (7)	20	11.5
Acetone-d6	C_3D_6O	64.12	0.872	–93.8	55.5	1.3554	20.7	2.05 (5)	2.2	29.92 (7) 206.68 (13)	19.4 0.9	2.84/ 2.81
Acetonitrile-d3	C_2D_3N	44.07	0.844	–46	80.7	1.3406	37.5	1.94 (5)	2.5	1.39 (7) 118.69	21	2.12
Benzene-d6	C_6D_6	84.15	0.950	6.8	79.1	1.4986	2.3	7.16		128.39 (3)	24.3	0.4
Chloroform-d1	$CDCl_3$	120.38	1.500	–64.1	60.9	1.4445	4.8	7.24		77.23 (3)	32	1.55
Cyclohexane-d12	$C_6D_{12}O$	96.24	0.890	7	78		2	1.38		26.43 (5)	19	0.80
Deuterium oxide	D_2O	20.03	1.107	3.8	101.4	1.328	78.5	4.81				
1,2-Dichloroethane-d4	$C_2D_4Cl_2$	102.99	1.307	–35	83	1.443		3.72 (5)		43.6 (5)	23.5	
Dichloromethane-d2	CD_2Cl_2	86.95	1.362	–97	39.5	1.362		5.32 (3)	1.1	54 (5)	27.2	1.52
Diethylether-d10	$C_4D_{10}O$	84.19	0.78	–116.3	34.6			3.34 (m) 1.07 (m)		65.3 (5) 14.5 (7)	21 19	
Diethylene glycol dimethyl ether-d14 (diglyme-d14)	$C_6D_{14}O_3$	148.26	0.95	–68	162			3.49 (br) 3.40 (br) 3.22 (5)	1.5	70.7 (5) 70 (5) 57.7 (7)	21 21 21	
1,2-Dimethoxyethane-d10 (glyme-d10)	$C_4D_{10}O_2$	100.18	0.86	–58	83			3.40 (m) 3.22 (5)	1.6	71.7 (5) 57.8 (7)	21 21	
N,N-Dimethyl-formamide-d7	C_3D_7NO	80.14	1.04	–60	153	1.428	36.7	8.03 2.92 (5) 2.75 (5)	1.9 1.9	163.15 (3) 34.89 (7) 29.76 (7)	29.4 21.0 21.1	3.45
Dimethyl sulfoxide-d6	C_2D_6OS	84.17	1.190	20.2	190	1.4758	46.7	2.50 (5)	1.9	39.51 (7)	21.0	3.3
1,4-Dioxane-d6	$C_4D_8O_2$	96.16	1.129	12	99	1.4198	2.2	3.53 (m)		66.66 (5)	21.9	2.4
Ethanol-d6	C_2D_6O	52.11	0.888	–114.5	78	1.358	24.5	5.29 3.56 1.11 (m)		56.96 (5) 17.31 (7)	22 19	5.2
Methanol-d4	CD_4O	36.07	0.89	–99	65	1.3256	32.7	4.87 3.31 (5)	1.7	49.15 (7)	21.4	4.86
Methyl cyclohexane-d14	C_7D_{14}	112.27	0.77	–126	101	1.4189						
Nitrobenzene-d5	$C_6D_5NO_2$	128.14	1.253	6	211	1.5498		8.11 (br) 7.67 (br) 7.50 (br)		148.6 134.8 (3) 129.5 (3) 123.5 (3)	24.5 25 26	2.42
Nitromethane-d3	CD_3NO_2	64.06	1.19	–26	100	1.3795		4.33 (5)		62.8 (7)	22	2.2
2-Propanol-d8	C_3D_8O	68.15	0.786	–89.5	82.4	1.3728		5.12 3.89 (br) 1.10 (br)		62.9 (3) 24.2 (7)	21.5 19	
Pyridine-d5	C_5D_5N	84.13	1.02	–41	114	1.5079	12.4	8.74 7.58 7.22		150.35 (3) 135.91 (3) 123.87 (3)	27.5 24.5 25	4.97
Tetrachloroethane-d2	$C_2D_2Cl_4$	169.86	1.7	–43	146	1.493		5.91 (5)		74.2 (5)		1.5
Tetrahydrofuran-d8	C_4D_8O	80.16	0.99	–108	64	1.4035	7.6	3.58 1.73		67.57 (5) 25.37 (5)	22.2 20.2	2.42
Toluene-d8	C_7D_8	100.19	0.94	–85	109	1.4932	2.4	7.09 (m) 7.00 6.98 (m) 2.09 (5)	2.3	137.86 129.24 (3) 128.33 (3) 125.49 (3) 20.4 (7)	23 24 24 19	0.45
2,2,2-Trifluoroacetic Acid-d1	$C_2DF_3O_2$	115.03	1.50	–15	71	1.30		11.50		164.2 (4) 116.6 (4)		11.5
2,2,2-Trifluoroethanol-d3	$C_2D_3F_3$	87.06	1.42	–44	77	1.30		5.02 3.88 (4x3)	2 (9)	126.3 (4) 61.5 (4x5)	22	5

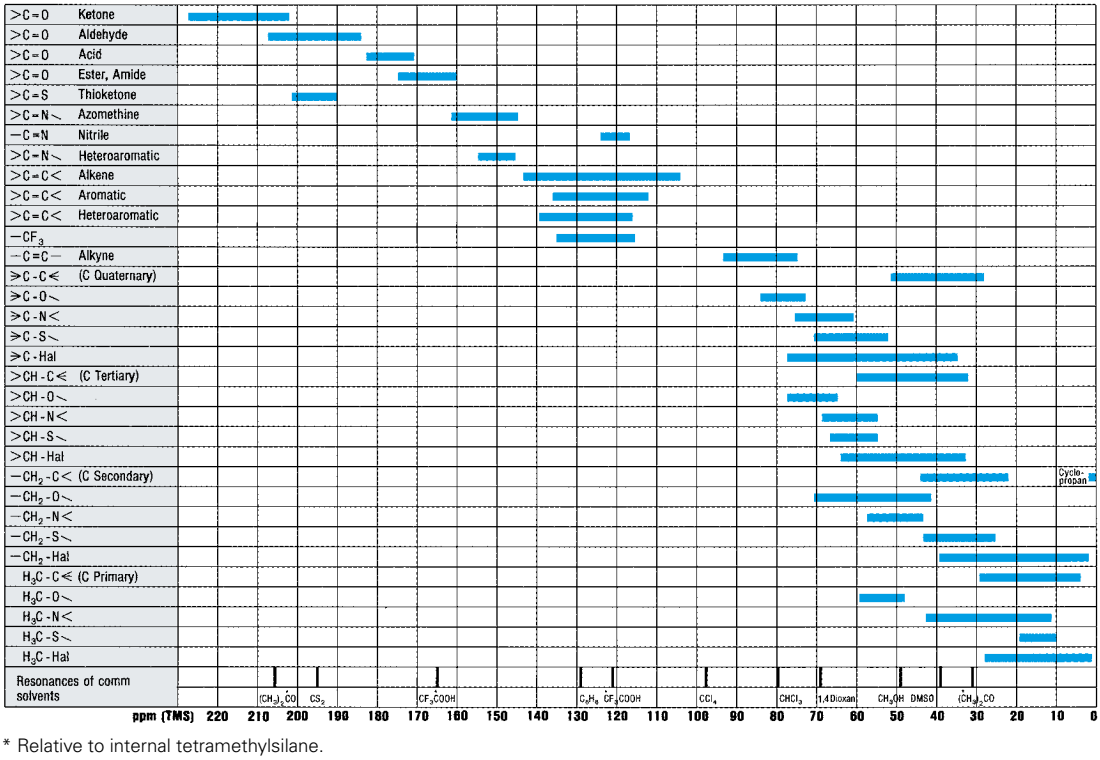
This Table summarizes the physical properties of deuterated solvents and the chem. shifts (rel. to TMS) and deuterium couplings for the solvent signals and the approximate shifts for residual water (last column).

NMR Tables

^{1}H Chemical Shifts in Organic Compounds



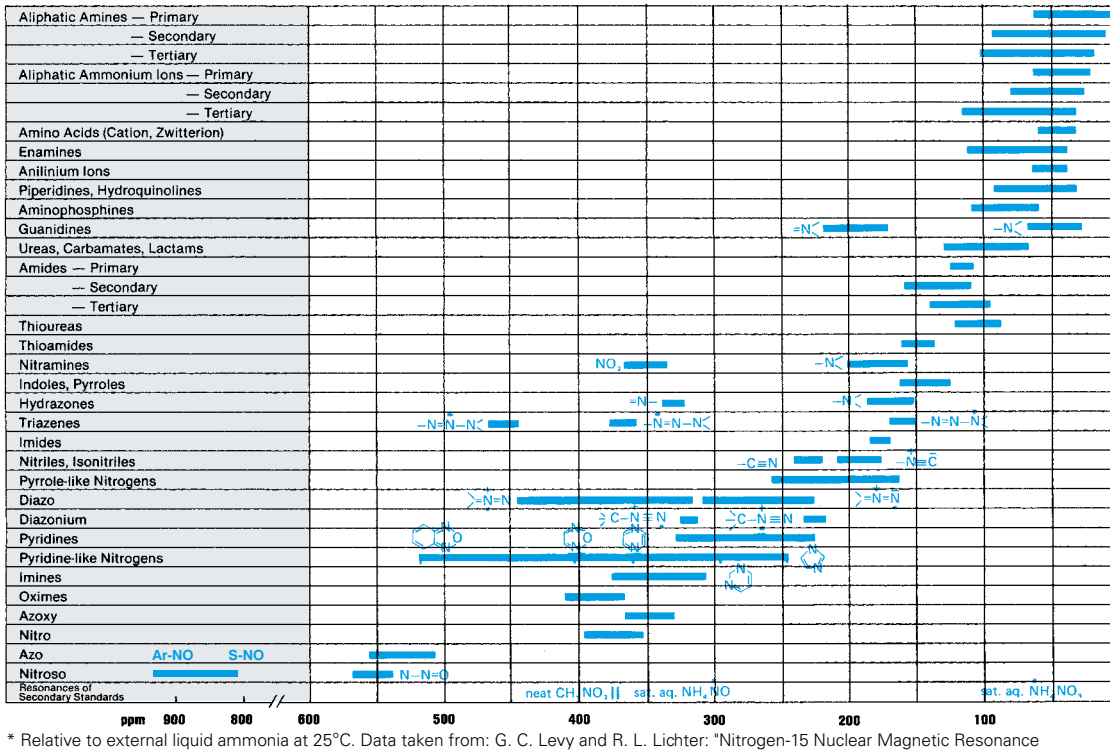
^{13}C Chemical Shifts in Organic Compounds*



* Relative to internal tetramethylsilane.

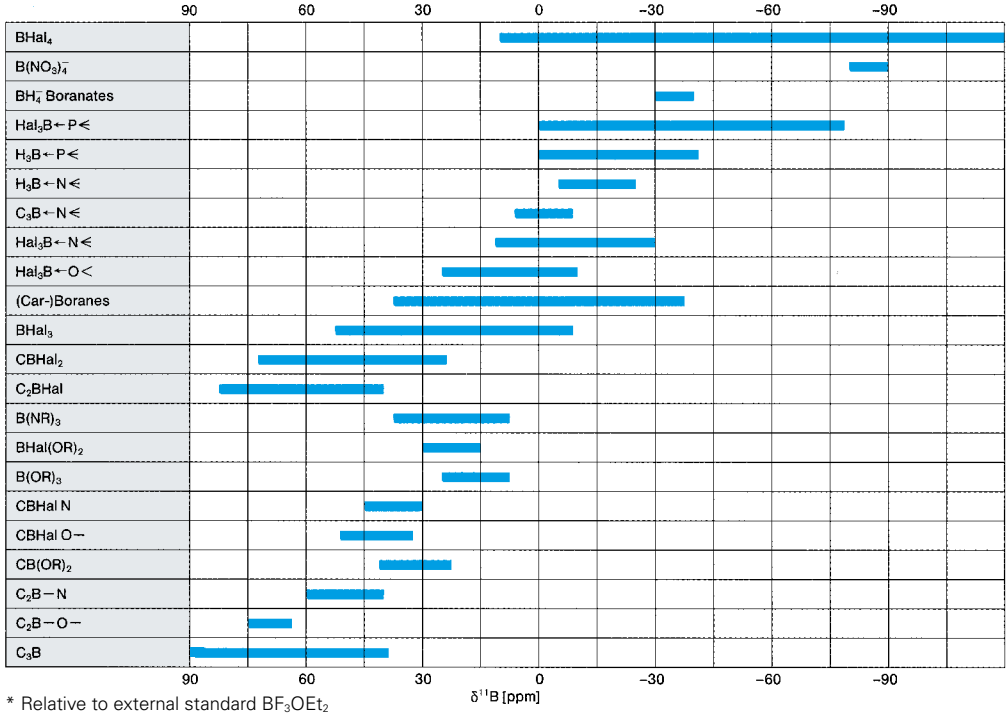
NMR Tables

^{15}N Chemical Shifts in Organic Compounds*



* Relative to external liquid ammonia at 25°C. Data taken from: G. C. Levy and R. L. Lichter: "Nitrogen-15 Nuclear Magnetic Resonance Spectroscopy", J. Wiley, 1979.

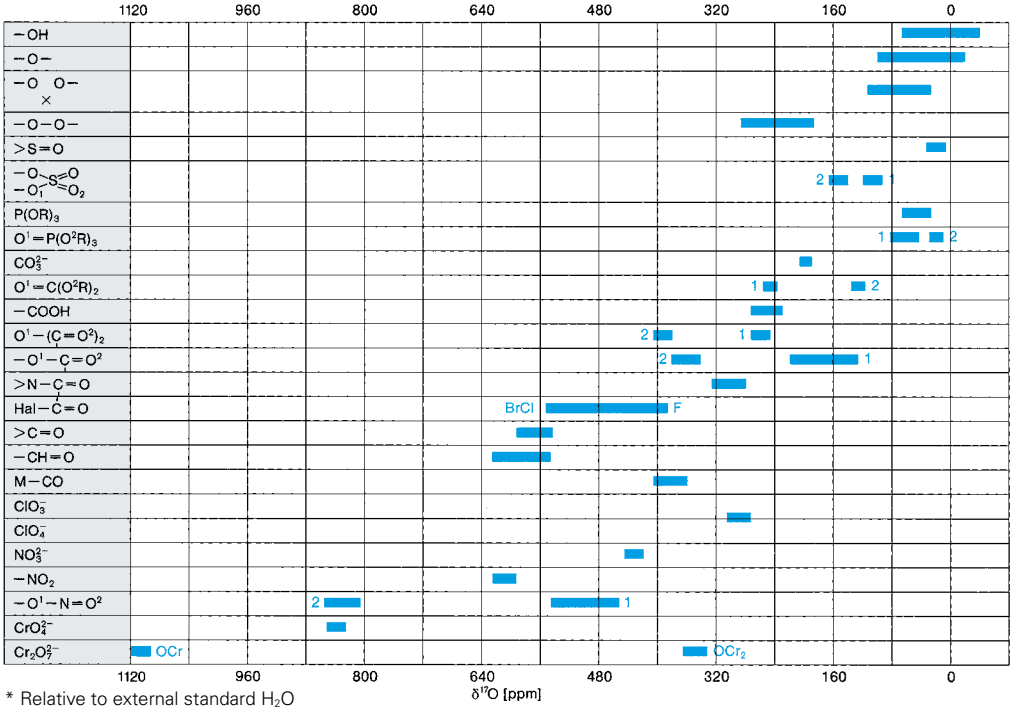
^{11}B Chemical Shifts*



* Relative to external standard BF_3OEt_2

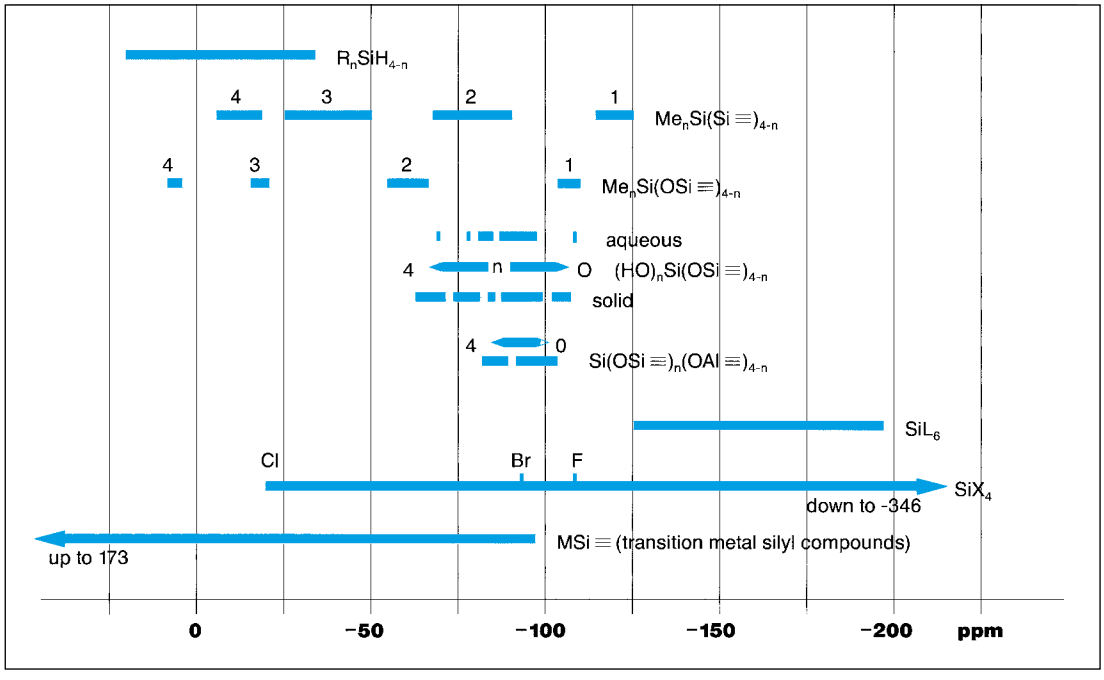
NMR Tables

^{17}O Chemical Shifts*



* Relative to external standard H_2O

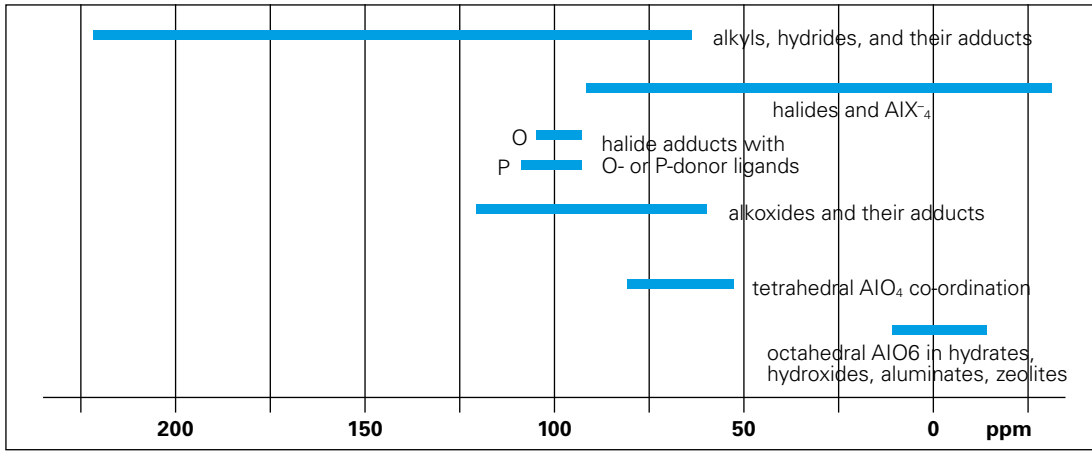
^{29}Si Chemical Shifts*



* Relative to $Si(CH_3)_4$.

NMR Tables

^{27}Al Chemical Shifts*



* Relative to $Al(H_2O)^{3+}_6$.

MRI Tables

Abbreviations and Acronyms Used in Magnetic Resonance Imaging

Method	Description	Equivalent acronyms
SINGLEPULSE	Basic pulse-and-acquire spectroscopy	FID
NSPECT	Non-localized spectroscopy with NOE and decoupling options	FID
CSI	Chemical shift imaging with optional PRESS localization	
PRESS	Localized MRS with double spin echo	
STEAM	Localized MRS with stimulated echo (for short TE)	
ISIS	Localized MRS with inversion-based voxel definition	OSIRIS
DtiEpi	Diffusion tensor imaging with EPI (SE and STE)	PGSE-EPI
DtiStandard	Diffusion tensor imaging with 2DFT (SE and STE)	PGSE
EPI	Echo-Planar Imaging (GE and SE), single-shot or interleaved, with navigator-based phase stabilization and automatic ghost correction	
FAIR_EPI	Pulsed arterial spin labelling-based perfusion imaging with EPI	
FC2D_ANGIO	Time-of-flight angiography flow-compensated	TOF-angio
FL2D_ANGIO	Time-of-flight angiography w/o flow-comp. (short TE)	
FISP	Fast gradient echo with steady state signal selection (FID, echo or fully balanced), and optional inversion recovery for T1 mapping.	FLASH, FAST, FISP, PSIF, CE-FAST, SSFP, GRASS, TrueFISP
FLASH	Gradient echo	FISP, GRASS, FAST
GEFC	Gradient echo with flow compensation	
MDEFT	T1-weghted hi-res imaging with inversion-recovery preparation	MPRAGE
MGE	Multiple gradient echo	
MSME	Multiple spin echo including T2 mapping	
RARE	Fast spin echo based on CPMG sequence	FSE, TSE
RAREVTR	RARE with variable TR for simultaneous T1&T2 mapping	
RAREst	Fast spin echo for short TE using slew-rate-optimized gradients	HASTE
FLOW_MAP	Quantitative flow mapping and PC-angio	
UTE	Ultra-short TE radial scan	
FieldMap	Quantitative B0 mapping, part of the MAPSHIM tool for localized high-order shimming	
SPIRAL	Fast MRI with spiral k-space scan	
IntraGate-FLASH	Cardiac and respiration-cine with retrospective (trigger-free) gating	

NMR Tables

Additivity Parameters for ^{13}C Chemical Shifts in Substituted Benzenes

$\delta_i = 128.5 + S_i(\delta_i)$, $S_i(\delta_i)$ refers to the carbon atom bearing the substituent

Substituent	$S_i(\delta_i)$	$S_i(\delta_o)$	$S_i(\delta_m)$	$S_i(\delta_p)$	Substituent	$S_i(\delta_i)$	$S_i(\delta_o)$	$S_i(\delta_m)$	$S_i(\delta_p)$
–H	0.0	0.0	0.0	0.0	**–I**	–32.3	9.9	2.6	–0.4
–CH_3	9.3	0.6	0.0	–3.1	**–OH**	26.9	–12.7	1.4	–7.3
–CH_2CH_3	15.7	–0.6	–0.1	–2.8	**–OCH_3**	30.2	–14.7	0.9	–8.1
–$CH(CH_3)_2$	20.1	–2.0	0.0	–2.5	**–NH_2**	19.2	–12.4	1.3	–9.5
–$C(CH_3)_3$	22.1	–3.4	–0.4	–3.1	**–$N(CH_3)_2$**	22.4	–15.7	0.8	–11.8
–Cyclopropyl	15.1	–3.3	–0.6	–3.6	**–$N(C_6H_5)_2$**	19.3	–4.4	0.6	–5.9
–CH_2Cl	9.1	0.0	0.2	–0.2	**–NO_2**	19.6	–5.3	0.8	6.0
–CH_2Br	9.2	0.1	0.4	–0.3	**–CN**	–16.0	3.5	0.7	4.3
–CF_3	2.6	–2.2	0.3	3.2	**–NCO**	5.7	–3.6	1.2	–2.8
–CH_2OH	13.0	–1.4	0.0	–1.2	**–$SC(CH_3)_3$**	4.5	9.0	–0.3	0.0
–$CH=CH_2$	7.6	–1.8	–1.8	–3.5	**–COH**	9.0	1.2	1.2	6.0
–C≡CH	–6.1	3.8	0.4	–0.2	**–$COCH_3$**	9.3	0.2	0.2	4.2
–C_6H_5	13.0	–1.1	0.5	–1.0	**–COOH**	2.4	1.6	–0.1	4.8
–F	35.1	–14.3	0.9	–4.4	**–COO^-**	7.6	0.8	0.0	2.8
–Cl	6.4	0.2	1.0	–2.0	**–$COOCH_3$**	2.1	1.2	0.0	4.4
–Br	–5.4	3.3	2.2	–1.0	**–COCl**	4.6	2.9	0.6	7.0

Some Representative ^{19}F Chemical Shifts Referenced to $CFCl_3$

	δ / ppm		δ / ppm		δ / ppm
MeF	-271.9	$CFBr_3$	7.4	$FCH=CH_2$	-114
EtF	-213	CF_2Br_2	7	$F_2C=CH_2$	-81.3
CF_2H_2	-1436	CFH_2Ph	-207	$F_2C=CF_2$	-135
CF_3R	-60 to -70	CF_2Cl_2	-8	C_6F_6	-163
AsF_5	-66	$[AsF_6]^-$	-69.5	$[BeF_4]^-$	-163
BF_3	-131	ClF_3	116; -4	ClF_5	247; 412
IF_7	170	MoF_6	-278	ReF_7	345
SeF_6	55	$[SbF_6]^-$	-109	SbF_5	-108
$[SiF_6]^{2-}$	-127	TeF_6	-57	WF_6	166
XeF_2	258	XeF_4	438	XeF_6	550

Some Representative ^{31}P Chemical Shifts Referenced to 85 % H_3PO_4

(a) Phosphorus (III) compounds

	δ / ppm		δ / ppm
PMe_3	-62	$PMeF_2$	245
PEt_3	-20	$PMeH_2$	-163.5
P(*n*-Pr)$_3$	-33	$PMeCl_2$	192
P(*i*-Pr)$_3$	-19.4	$PMeBr_2$	184
P(*n*-Bu)$_3$	-32.5	PMe_2F	186
P(*i*-Bu)$_3$	-45.3	PMe_2H	-99
P(*s*-Bu)$_3$	7.9	PMe_2Cl	96.5
P(*t*-Bu)$_3$	63	PMe_2Br	90.5

(b) Phosphorus (V) compounds

	δ / ppm		δ / ppm
Me_3PO	36.2	Me_3PS	59.1
Et_3PO	48.3	Et_3PS	54.5
$[ME_4P]^+$	24.4	$[Et_4P]^+$	40.1
$[PO_4]^{3-}$	6.0	$[PS_4]^{3-}$	87
PF_5	-80.3	$[PF_6]^-$	-145
PCl_5	-80	$[PCl_4]^+$	86
$MePF_4$	-29.9	$[PCl_6]^-$	-295
Me_3PF_2	-158	Me_2PF_3	8.0

NMR Tables

Some Important Silylated Compounds Used as ^{1}H Shift References

Name	Chemical formula	Abbre-viation	Mole-cular weigth	Boiling or melting point (°C)	δ ^{1}H ppm rel. TMS
Tetramethylsilane	$(CH_3)_4Si$	TMS	88.2	BP = 26.3	0
Hexamethyldisilane	$(CH_3)_3Si–Si(CH_3)_3$	HMDS	146.4	BP = 112.3	0.037
Hexamethyldisiloxane	$(CH_3)_3Si–O–Si(CH_3)_3$	HMDSO	162.4	BP = 100	0.055
Hexamethyldisilazane	$(CH_3)_3Si–NH–Si(CH_3)_3$	HMDSA	161.4	BP = 125	0.042
3-(trimethylsilyl)propane sulfonic acid soduim salt 4,4-dimethyl-4-silapentane sodium sulfonate	$(CH_3)_3Si(CH_2)_3SO_3Na$	TSPSA DSS	218.3	MP = 200	0.015
3-(trimethylsilyl)propionic acid sodium salt 4,4-dimethyl-4-silapentane sodium carboxylate	$(CH_3)_3Si(CH_2)_2COONa$	TSP DSC	168.2	MP > 300	0.000
3-(trimethylsilyl) 2,2,3,3-tetra-deuteropropionic acid sodium salt	$(CH_3)_3Si(CD_2)_2COONa$	TSP-d_4	172.2	MP > 300	0.000
Octamethylcyclotetrasiloxane	$(CH_3)_2Si[O–Si(CH_3)_2]_3–O$	OCTS	296.8	BP = 175 MP = 16.8	0.085
1,1,3,3,5,5-hexakis-(trideutero-methyl)-1,3,5-trisilacyclohexane	$(CD_3)_2Si(–CH_2–Si(CD_3)_2–CH_2)_2$	CS-d_{18}	216.6	BP = 208	-0.327
Tetrakis-(trimethylsilyl)-methane	$[(CH_3)_3Si]_4C$	TTSM	304.8	MP = 307	0.236

Enhancement Factors η_{NOE} and η_{INEPT} for X {^{1}H} Nuclear Overhauser and INEPT Experiments

X	^{19}F	^{31}P	^{11}B	^{13}C	^{15}N	^{29}Si	^{57}Fe	^{103}Rh	^{109}Ag	^{119}Sn	^{183}W
η_{NOE}[a]	0.53	1.24	1.56	1.99	–4.93	–2.52	15.41	–15.80	–10.68	–1.33	11.86
η_{INEPT}[b]	1.06	2.47	3.12	3.98	–9.86	–5.03	30.82	–31.59	–21.37	–2.67	23.71

[a] The maximum possible intensity enhancement is equal to 1 + η_{NOE} in the extreme narrowing limit.
[b] For ^{19}F or ^{31}P as polarization source (irradiated nucleus) the factors η_{NOE} and η_{INEPT} are reduced by the factor 0.941 [$\gamma(^{19}F)/\gamma(^1H)$] and 0.405 [$\gamma(^{31}P)/\gamma(^1H)$]

Relevant Properties of Cryogenic Fluids

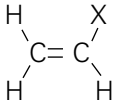
(Liquid helium and nitrogen are used in supercon magnets)

Cryogen	Normal Boiling Point (K)	Latent Heat (J/g)	Amount of Liquid Evaporated by 1 Watt (l/hour)	Liquid Density (g/ml)	Gas Density at NTP (g/ml)	Liquid to NTP Gas Volume Ratio	Enthalpy Change (gas) B.P. to 77 K (J/mole)	Enthalpy Change (gas) 77 to 300 K (J/mole)
Liquid Helium	4.2	20.9	1.038	0.125	1.79×10^{-4}	1 : 700	384	1157
Liquid Hydrogen	20.39	443	0.115	0.071	8.99×10^{-5}	1 : 790	590	2900
Liquid Nitrogen	77.55	198	0.023	0.808	1.25×10^{-3}	1 : 650	–	234
Liquid Oxygen	90.19	212.5	0.015	1.014	1.43×10^{-3}	1 : 797	–	From BP: 193

NTP = normal room temperature and atmospheric pressure

NMR Tables

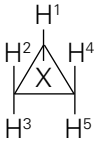
^{1}H, ^{1}H Coupling Constants in Selected Organic Molecules



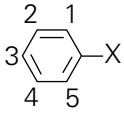
X	$^3J_{cis}$	$^3J_{trans}$	^2J
H	11.6	19.1	2.5
Li	19.3	23.9	7.1
COOH	10.2	17.2	1.7
CN	11.75	17.92	0.91
C_6H_5	11.48	18.59	1.08
CH_3	10.02	16.81	2.08
OCH_3	7.0	14.1	-2.0
Cl	1.3	14.6	-1.4
Br	7.1	15.2	-1.8
F	4.65	12.75	-3.2

$H_3C\text{-}CH_2\text{-}X$

X	^3J
Li	8.90
$Si(C_2H_5)_3$	8.0
H	7.5
C_6H_5	7.62
CN	7.60
I	7.45
Br	7.33
CH_3	7.26
Cl	7.23
$N(C_2H_5)_2$	7.13
OC_2H_5	6.97
$^+O(C_2H_5)_2$	4.7



X	$^3J(1,2)$	$^3J(1,3)$	$^3J(2,4)$	$^3J(3,5)$	$^3J(2,5)$	$^2J(2,3)$
H	8.97	5.58	8.97	8.97	5.58	-4.34
Cl	7.01	3.58	10.26	10.58	7.14	-6.01
Br	7.13	3.80	10.16	10.45	7.01	-6.12
I	7.51	4.37	9.89	9.97	6.63	-5.94
NH_2	6.63	3.55	9.65	9.89	6.18	-4.29
CN	8.43	5.12	9.18	9.49	7.08	-4.72
COOH	8.04	4.57	9.26	9.66	7.14	-4.00
COCl	7.88	4.43	9.19	9.99	7.59	-4.46
$COCH_3$	7.96	4.55	8.76	9.60	6.94	-3.41



X	$^3J(1,2)$	$^4J(1,3)$	$^5J(1,4)$	$^4J(1,5)$	$^3J(2,3)$	$^4J(2,4)$
H	7.54	1.37	0.66	1.37	7.54	1.37
Li	6.73	1.54	0.77	0.74	1.42	1.29
CH_3	7.64	1.25	0.60	1.87	7.52	1.51[a]
$COOCH_3$	7.86	1.35	0.63	1.79	7.49	1.31
I	7.93	1.14	0.47	1.88	7.47	1.75
Br	8.05	1.12	0.46	2.1	7.44	1.78
Cl	8.05	1.13	0.48	2.27	7.51	1.72
NH_2	8.02	1.11	0.47	2.53	7.39	1.60
$N(CH_3)_2$	8.40	1.01	0.43	2.76	7.29	1.76
$N(CH_3)_3$	8.55	0.92	0.48	3.05	7.46	1.69
NO_2	8.36	1.18	0.55	2.40	7.47	1.48
OH	8.17	1.09	0.49	2.71	7.40	1.74
OCH_3	8.30	1.03	0.44	2.94	7.36	1.76
F	8.36	1.07	0.43	2.74	7.47	1.82[b]

[a] $^4J(1, CH_3)$ -0.75
$^5J(2, CH_3)$ 0.36
$^6J(3, CH_3)$ -0.62

[b] $^3J(1, F)$ 8.91
$^4J(2, F)$ 5.69
$^5J(3, F)$ 0.22

Substituent Effect S(*i,j*) for J_{HH} in Monosubstituted Benzenes

pos. *i,j*	F	Cl	Br	I	NO_2	OCH_3
1,2	+0.81	+0.61	+0.53	+0.39	+0.77	+0.79
1,3	−0.34	−0.23	−0.27	−0.25	−0.20	−0.32
1,4	−0.24	−0.16	−0.20	−0.19	−0.16	−0.22
1,5	+1.21	+0.87	−0.71	+0.51	+1.02	+1.33
2,3	−0.04	+0.03	−0.05	−0.04	−0.07	−0.16
2,4	+0.39	+0.34	+0.36	+0.37	+0.08	+0.38

NMR Tables

Typical Stray Field Data for NMR Magnet Systems

Magnet System ^{1}H MHz/mm Bore	Axial Distance (m) from Magnet Center to 5 Gauss (0.5 mT) Line	Radial Distance (m) from Magnet Center to 5 Gauss (0.5 mT) Line
200 MHz/154 mm US PLUS LH	1.80	0.90
300 MHz/54 mm US LH	0.90	0.60
300 MHz/54 mm Fourier US LH	0.90	0.60
300 MHz/54 mm Ascend ULH	0.90	0.60
300 MHz/89 mm Ascend	1.10	0.55
300 MHz/154 mm US PLUS LH	2.00	1.00
400 MHz/54 mm Ascend	1.00	0.50
400 MHz/54 mm Ascend ULH	1.00	0.50
400 MHz/54 mm Ascend RS	1.00	0.50
400 MHz/89 mm Ascend	1.20	0.60
400 MHz/89 mm Ascend DNP	1.50	1.10
400 MHz/154 mm US PLUS LH	2.55	1.50
500 MHz/54 mm Ascend	1.20	0.60
500 MHz/54 mm Ascend ULH	1.20	0.60
500 MHz/54 mm Ascend RS	1.20	0.60
500 MHz/89 mm Ascend	1.20	0.60
500 MHz/154 mm US PLUS LH	2.55	1.50
600 MHz/54 mm Ascend	1.40	0.70
600 MHz/54 mm Ascend ULH	1.40	0.70
600 MHz/89 mm Ascend	2.00	1.00
600 MHz/89 mm Ascend DNP	2.00	1.00
700 MHz/54 mm Ascend	1.60	0.80
750 MHz/54 mm Ascend	2.00	1.00
750 MHz/89 mm Ascend	2.80	1.40
800 MHz/54 mm Ascend	2.50	1.50
850 MHz/54 mm Ascend	2.70	1.60
850 MHz/89 mm US^{2} WB	4.60	3.30
900 MHz/54 mm US^{2}	4.60	3.30
900 MHz/89 mm US^{2} WB	4.60	3.30
950 MHz/54 mm US^{2}	4.60	3.30
1000 MHz/54 mm UltraStabilized	15.00	12.00

LH = Long Hold, ULH = Ultra Long Hold

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

2D	Two-Dimensional
3D	Three-Dimensional
ACCORDION	2D technique, simultaneous incrementing of evolution and mixing times
ADA	**A**lternated **D**elay **A**cquisition
ADC	**A**nalog-to-**D**igital **C**onverter, **A**pparent **D**iffusion **C**onstant
ADEQUATE	**A**stonishingly Sensitive **DoublE QUA**ntum **T**ransfer **E**xperiment
ADLF	**A**diabatic **D**emagnetization in the **L**aboratory **F**rame
ADRF	**A**diabatic **D**emagnetization in the **R**otating **F**rame
A.E.COSY	**A**lternative **E**xclusive **COSY**
AFP	**A**diabtic **F**ast **P**assage
AHT	**A**verage **H**amiltonian **T**heory
AJCP	**A**diabatic **J** **C**ross **P**olarization
AMCP	**A**mplitude-**M**odulated **C**ross **P**olarization
ANGIO	MR **ANGIO**graphy
APHH-CP	**A**diabatic-**P**assage **H**artmann-**H**ahn **C**ross **P**olarization
APT	**A**ttached **P**roton **T**est
AQ	**A**c**Q**uisition
ARP	**A**diabatic **R**apid **P**assage
ASIS	**A**romatic **S**olvent-**I**nduced **S**hift
ASL	**A**rterial **S**pin **L**abeling
ASTM	**A**merican **S**ociety for **T**esting and **M**aterials
BASE	**BA**sis imaging with **SE**lective-inversion preparation
BB	**B**road**B**and, as in decoupling
BDR	**B**roadband **D**ipolar **R**ecoupling
bEPI	**b**lipped **EPI**
bFFE	**b**alanced **F**ast-**F**ield **E**cho
BIRD	**BI**linear **R**otation **D**ecoupling
BIRD/2	half **BIRD**, bilinear π**/2** pulse
BLEW	A windowless multiple-pulse decoupling sequence
BLEW-*n*	**B**urum-**L**inder-**E**rnst **W**indowless homonuc. dipolar dec. sequence of ***n*** pulses
BMS	**B**ulk **M**agnetic **S**usceptibility
BOLD	**B**lood **O**xygenation **L**evel-**D**ependent contrast (MRI)
BOSS	**B**im**O**dal **S**lice-**S**elective
BP	**BiP**hasic
BPP	**B**loembergen/**P**urcell/**P**ound (theory)
BR-*n*	**B**urum-**R**him homonuclear dipolar decoupling sequence of ***n*** pulses
BSP	**B**loch-**S**iegert **P**hase
BURP	**B**and-selective **U**niform **R**esponse **P**ure-phase pulse
bTFE	**b**alanced **T**urbo **F**ield **E**cho
BW	**B**and**W**idth
BWR	**B**loch-**W**angsness-**R**edfield theory
CA	**C**ontrast **A**gent
CAMELSPIN	**C**ross-relaxation **A**ppropriate for **M**inimolecules **E**mulated by **L**ocked **SPIN**s
CBCA(CO)NH	**C**$\boldsymbol{\beta}$(*i*-1) and **C**$\boldsymbol{\alpha}$(*i*-1), **N**(*i*), H_N(*i*) 3D correl.
CBCANH	**C**$\boldsymbol{\beta}$(*i*,*i*-1) and **C**$\boldsymbol{\alpha}$(*i*,*i*-1), **N**(*i*), H_N(*i*) 3D correl.
CCPPA	**C**oupled **C**luster **P**olarization **P**ropagator **A**pproximation
CE	**C**ontrast-**E**nhanced
CEST	**C**hemical **E**xchange **S**aturation **T**ransfer
CH-COSY	**C**arbon-**H**ydrogen **CO**rrelation **S**pectroscop**Y**
CHESS	**CHE**mical **S**hift **S**elective Imaging Sequence
CHIRP	rf pulse with linear freq. modulation
CIDEP	**C**hemically **I**nduced **D**ynamic **E**lectron **P**olarization
CIDNP	**C**hemically **I**nduced **D**ynamic **N**uclear **P**olarization
CINE	"movie-like" MRI
CISS	**C**onstructive **I**nterference **S**teady **S**tate
CNR	**C**ontrast-to-**N**oise **R**atio
COLOC	**CO**rrelated Spectroscopy via **LO**ng-Range **C**oupling
COLOC-S	**COLOC** with **S**uppression of one-bond correlations
CONOESY	**C**ombined **COSY/NOESY**
CORMA	**CO**mplete **R**elaxation **M**atrix **A**nalysis
CORY-*n*	**CORY** modification of **BR-*n***
COSS	**CO**rrelation with **S**hift **S**caling
COSY	**CO**rrelated **S**pectroscop**Y**
COSY-45	**COSY** with **45°** mixing pulse
COSYDEC	**COSY** with F_1 **DEC**oupling
COSYLR	**COSY** for **L**ong-**R**ange couplings
CP	**C**ross **P**olarization**,** **C**ircular **P**olarization
CPD	**C**omposite-**P**ulse **D**ecoupling
CPMAS	**C**ross **P**olarization **M**agic-**A**ngle **S**pinning
CPMG	**C**arr-**P**urcell-**M**eiboom-**G**ill Sequence
CRAMPS	**C**ombined **R**otation **A**nd **M**ultiple **P**ulse **S**pectroscopy
CRAZED	**C**orrelated Spectroscopy **R**evamped by **A**symmetric **Z**-gradient **E**cho **D**etection
CRINEPT	**C**ross-correlated **R**elaxation-enhanced **INEPT**
CS	**C**ontiguous **S**lice
CSA	**C**hemical **S**hift **A**nisotropy
CSCM	**C**hemical **S**hift **C**orrelation **M**ap
CSI	**C**hemical **S**hift **I**maging
CT	**C**onstant **T**ime
CW	**C**ontinuous **W**ave
CYCLCROP	**CYCL**ic **CRO**ss **P**olarization
CYCLOPS	**CYCL**ically **O**rdered **P**hase **S**equence
CYCLPOT	**CYCL**ic **PO**larization **T**ransfer
DAC	**D**igital-to-**A**nalog **C**onverter
DAISY	**D**irect **A**ssignment **I**nterconnection **S**pectroscop**Y**
DANTE	**D**elay **A**lternating with **N**utation for **T**ailored **E**xcitation
DAS	**D**ynamic **A**ngle **S**pinning
DCNMR	NMR in Presence of an Electric **D**irect **C**urrent
DD	**D**ipole-**D**ipole
DE	**D**ual **E**cho**,** **D**riven **E**quilibrium

Abbreviations and Acronyms Used in Magnetic Resonance

DECSY	**D**ouble-quantum **E**cho **C**orrelated **S**pectroscop**Y**
DEFT	**D**riven **E**quilibrium **F**ourier **T**ransform
DEPT	**D**istortionless **E**nhancement by **P**olarization **T**ransfer
DEPTH	spin-echo sequence for spatial localization
DEPTQ	**DEPT** including quaternary carbons
DFT	**D**iscrete **F**ourier **T**ransformation
DICE	**DI**rect **C**onnectivity **E**xperiment
DICOM	**D**igital **I**maging and **CO**mmunications in **M**edicine
DIGGER	**D**iscreet **I**solation from **G**radient-**G**overned **E**limination of **R**esonances
DIPSI	Composite-pulse **D**ecoupling **I**n the **P**resence of **S**calar **I**nteractions
DISCO	**DI**fferences and **S**ums within **CO**SY
DLB	**D**ifferential **L**ine **B**roadening
DNMR	**D**ynamic **NMR**
D.NOESY	**D**irect cross-relaxation **NOESY**
DNP	**D**ynamic **N**uclear **P**olarization
DOC	**D**ouble **CO**nstant-Time sequence
DOPT	**D**ipolar **O**rder **P**olarization **T**ransfer
DOR	**D**ouble-**O**rientation **R**otation
DOSY	**D**iffusion-**O**rdered **S**pectroscop**Y**
DOUBTFUL	**DOUB**le Quantum **T**ransition for **F**inding **U**nresolved **L**ines
DPFGSE	**D**ouble **P**ulsed **F**ield **G**radient **S**pin **E**cho
DQ	**D**ouble **Q**uantum
DQC	**D**ouble **Q**uantum **C**oherence
DQF	**D**ouble **Q**uantum **F**ilter
DQF-COSY	**D**ouble **Q**uantum **F**iltered **COSY**
DQSY	**D**ouble-**Q**uantum CO**SY**
DQ/ZQ	**D**ouble **Q**uantum/**Z**ero **Q**uantum Spectroscopy
DRAMA	**D**ipolar **R**ecovery **A**t the **M**agic **A**ngle
DREAM	**D**ouble-quantum **R**elay **E**nhancement by **A**diabatic **M**ixing
DRESS	**D**epth **RES**olved **S**pectrosocpy
DRIVE	**DRIV**en **E**quilibrium
DRYCLEAN	**D**iffusion-**R**educed water signals in spectroscop**Y** of mole**C**ules moving s**L**ow**E**r th**AN** water
DSA	**D**ata-**S**hift **A**cquisition
DSC	**D**ynamic **S**usceptibility **C**ontrast
DSE	**D**ual **S**pin **E**cho
DTI	**D**iffusion **T**ensor **I**maging
DTRCF	**D**ouble **T**ilted **R**otating **C**oordinate **F**rame
DTSE	**D**ouble **T**urbo **S**pin **E**cho
DUMBO	**D**ecoupling **U**sing **M**ind-**B**oggling **O**ptimization – a numerically optimized phase-modulated homonuc. dipolar dec. sequence
DWI	**D**iffusion-**W**eighted **I**maging
E-BURP	**E**xcitation **BURP** pulse
EC	**E**ddy **C**urrents
E.COSY	**E**xclusive **CO**rrelation **S**pectroscop**Y**
ECO-WURST	**WURST** decoupling with **E**limination of **C**ycling **O**scillations
EFG	**E**lectric **F**ield **G**radient
EM	**E**xponential **M**ultiplication
EMF	**E**lectro**M**agnetic **F**ield **E**lectro**M**otive **F**orce
ENDOR	**E**lectron-**N**uclear **DO**uble **R**esonance
ENMR	**E**lectrophoretic **NMR**
EPI	**E**cho-**P**lanar **I**maging
EPR	**E**lectron **P**aramagnetic **R**esonance
EPS	**E**cho-**P**lanar **S**pectroscopy
ES, ESP	**E**cho **S**pacing
E-SHORT	**E**nhanced **SHORT** repetition MRI
ESR	**E**lectron **S**pin **R**esonace
E.TACSY	**E**xclusive **TACSY**
EXORCYCLE	4-step phase cycle for spin echoes
EXSY	**EX**change **S**pectroscop**Y**
FA	**F**lip **A**ngle
FADE	**FA**SE Acq. with **D**ouble **E**cho
FAIR	**F**low-sensitive **A**lternating **I**nversion **R**ecovery
FASE	**F**ast **A**dvanced **S**pin **E**cho
FAST	**F**ourier-**A**cquired **ST**eady State
FASTMAP	**FAST** B_0 Field **MAP**ping for shimming
FATE	**FA**st **T**urbo **E**cho
FC	**F**low **C**ompensation
FC2D_ANGIO	**F**low-**C**ompensated time-of-flight **2D ANGIO**graphy
FE	**F**ield **E**cho, **F**requency **E**ncoding
FFE	**F**ast **F**ield **E**cho
FFLG	**F**lip-**F**lop **L**ee-**G**oldburg decoupling
FFT	**F**ast **F**ourier **T**ransform
FGRE	**F**ast **G**radient-**R**ecalled **E**cho
FID	**F**ree **I**nduction **D**ecay
FIDS	**FI**tting of **D**oublets and **S**inglets
FieldMap	B_0 **Field Map**ping for localized shimming
FIRFT	**F**ast **I**nversion-**R**ecovery **F**ourier **T**ransform
FISP	**F**ast **I**maging with **S**teady-state **P**recession
FL2D_ANGIO	**FL**ow-sensitive **2D ANGIO**graphy
FLAIR	**FL**uid **A**ttenuation **I**nversion-**R**ecovery
FLASH	**F**ast **L**ow-**A**ngle **SH**ot imaging
FLOCK	Long-range HETCOR using 3 BIRD pulses
FLOPSY	**FI**ip-FI**OP S**pectroscop**Y**
FLOW_MAP	Quantitative **FLOW MAP**ping and PC-angiography
FMP	**F**ast **M**ulti**P**lanar
fMRI	**f**unctional **MRI**
FOCSY	**FO**ldover-**C**orrected **S**pectrospcop**Y**
FONAR	Field-focusing MRI
FOV	**F**ield **O**f **V**iew
FPT	**F**inite **P**erturbation **T**heory
FR	**F**requency **E**ncoding
FS	**F**at **S**aturation, **F**ast **S**can

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

FSE	**F**ast **S**pin **E**cho
FSLG	**F**requency-**S**witched **L**ee-**G**oldburg – a homonuc. dipolar dec. scheme
FSPGR	**F**ast **SP**oiled **GR**adient Echo
FT	**F**ourier **T**ransform
FUCOUP	**FU**lly **COUP**led Spectroscopy
FWHM	**F**ull (line) **W**idth at **H**alf **M**aximum
GARP	**G**lobaly Optimized **A**lternating Phase **R**ectangular **P**ulses
GE	**G**radient **E**cho
GEFC	**G**radient **E**cho with **F**low **C**ompensation
gem-COSY	**gem**inal-filtered **COSY**
GES	**G**radient-**E**cho **S**pectroscopy
GFE	**G**radient **F**ield **E**cho
GRASE	**GRA**dient and **S**pin **E**cho
GRASP	**GR**adient-**A**ccelerated **SP**ectroscopy
GRASS	**G**radient-**R**ecalled **A**cquisition in the **S**teady **S**tate
GRE	**G**radient-**R**ecalled **E**cho
GRECCO	**GR**adient-**E**nhanced **C**arbon **CO**upling
GROESY	**G**radient-Enhanced Selective 1D **ROESY**
GROPE	**G**eneralized compensation for **R**esonance **O**ffset and **P**ulse length **E**rrors
GS	**G**radient **S**pectroscopy
gs- ...	**g**radient-**s**elected ... (e.g. gs-COSY)
H,X-COSY	**H,X** shift correlation (X-detected)
HASTE	**H**alf-Fourier **A**cquisition **S**ingle-shot **T**urbo spin **E**cho
HBHA (CBCA CO) NH	**H**β(i-1) and **H**α(i-1), **N**(i), **H$_N$**(i) 3D correl.
HCACO	**H**α(i), **C**α(i), **C'O**(i) 3D correl.
HCACON	**H**α(i), **C**α(i), **C'O**(i), **N**(i+1) 4D correl.
HCA(CO)N	**H**α(i), **C**α(i), **N**(i+1) 3D correl.
HCA(CO) NNH	**H**α(i), **C**α(i), **N**(i+1), **H$_N$**(i+1) 4D correl.
HCANNH	**H**α(i), **C**α(i), **N**(i), **H$_N$**(i) 3D correl.
(H)CC(CO) NH	**C**α,β,...(i), **N**(i+1), **H$_N$**(i+1) 3D correl.
HCCH-COSY	**H**α(i), **C**α(i), **H**β(i) 3D correl.
HCCH-TOCSY	total correlation of side-chain H and C
HDQC	**H**eteronuclear **D**ouble-**Q**uantum **C**orrelation
HEED	**H**ahn spin-**E**cho **E**xtende**D** sequence
HET2DJ	**HET**eronuclear **2D J**-correlated
HETCOR	**HET**eronuclear **COR**relation Spectroscopy
HETLOC	**HET**eronuclear **LO**ng-range **C**ouplings
HEHAHA	**HE**teronuclear **HA**rtmann **HA**hn
HMBC	**H**eteronuclear **M**ultiple-**B**ond **C**orrelation
HMQ	**H**eteronuclear **M**ultiple-**Q**uantum
HMQC	**H**eteronuclear **M**ultiple-**Q**uantum **C**oherence
HMSC	**H**eteronuclear **M**ultiple- and **S**ingle-bond **C**orrelation
HNCA	**H$_N$**(i), **N**(i), **C**α(i) and **C**α(i-1) 3D shift correlation
HNCA-J	3D **HNCA** to measure $^3J(H_N,H\alpha)$
HN(CA)NNH	**H$_N$**(i), **N**(i), **N**(i+1) and **N**(i-1) 3D correl.
HN(CA)CO	**H$_N$**(i), **N**(i), **C'O**(i), and **C'O**(i-1) 3D shift correlation
H(N)CACO	**H$_N$**(i), **C**α(i), **C'O**(i) 3D shift correlation
HNCAHA	**H$_N$**(i), **N**(i), **C**α(i), **H**α(i) 4D shift correlation
HNCO	**H$_N$**(i), **N**(i), **C'O**(i-1) 3D shift correlation
HN(CO)CA	**H$_N$**(i), **N**(i), **C**α(i-1) 3D shift correlation
H(N)COCA	**H$_N$**(i+1), **C'O**(i), **C**α(i) 3D shift correlation
HN(CO) CAHA	**H$_N$**(i+1), **N**(i+1), **C**α(i), **H**α(i) 4D shift correlation
HOESY	**H**eteronuclear **O**verhauser **E**ffect **S**pectroscop**Y**
HOHAHA	**HO**monuclear **HA**rtmann-**HA**hn Spectroscopy
HORROR	double-quantum **HO**mo-nuclea**R RO**tary **R**esonance
HQQC	**H**eteronuclear **Q**uadruple-**Q**uantum **C**orrelation
HR	**H**igh **R**esolution
HRPA	**H**igher **R**andom **P**hase **A**pproximation
HS	**H**omo**S**poil
HSL	**H**eteronuclear **S**pin **L**ock
HSQC	**H**eteronuclear **S**ingle-**Q**uantum **C**oherence
HTQC	**H**eteronuclear **T**riple-**Q**uantum **C**orrelation
I-BURP	**I**nversion **BURP** pulse
ICE	**I**ndirect **C**onnectivity **E**xperiment
IDESS	**I**mproved **DE**pth **S**elective single surface coil **S**pectroscopy
IDR	**I**nverted **D**irect **R**esponse
IEPI	**I**nterleaved **EPI**
IFT	**I**nverse **FT**
IGLO	**I**ndividual **G**auge for different **L**ocalized **O**rbitals
INADE-QUATE	**I**ncredible **N**atural **A**bu-dance **DoublE QUA**natum **T**ransfer **E**xperiment
INAPT	**INEPT** with selective 1H excitation
INDOR	**IN**ternuclear **DO**uble **R**esonance
INEPT	**I**nsensitive **N**uclei **E**nhanced by **P**olarization **T**ransfer
INEPT+	**INEPT** with refocusing period for in-phase multiplets
INEPT-R	**INEPT R**efocused for 1H-dec. spectra
INSIPID	**IN**adequate **S**ensitivity **I**mprovement by **P**roton **I**ndirect **D**etection
IntraGate-FLASH	Cardiac and respiration cine MRI with retrospective (trigger-free) gating
INVERSE	H, X correlation via ^{1}H detection
IPAP	**I**n-**P**hase **A**nti-**P**hase (in 2D)
IR	**I**nversion-**R**ecovery
IRMA	**I**terative **R**elaxation **M**atrix **A**nalysis
ISECR	**I**n-pha**SE CR**oss peaks (method)

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

ISIS	**I**mage-**S**elected **I**n-vivo **S**pectroscopy (single-voxel)
IST	**I**rreducible **S**pherical **T**ensor
IVIM	**I**ntra**V**oxel **I**ncoherent **M**otion
JCP	**J C**ross-**P**olarization
J-mod	**J mod**ulation
JR	**J**ump-and-**R**eturn sequence (90_y-τ-90_{-y})
J-res	**J-res**olved 2D
LAS	**L**aboratory **A**xis **S**ystem
LASE	**L**ow-**A**ngle **SE**
LB	**L**ine **B**roadening (via EM)
LG	**L**orentz-**G**auss window function
LIS	**L**anthanide **I**nduced **S**hift
LORG	**L**ocal **OR**i**G**in
LOSY	**LO**calized **S**pectroscop**Y**
LP	**L**inear **P**olarization, **L**inear **P**rediction
LPSVD	**L**inear **P**rediction using **S**ingular **V**alue **D**ecomposition
LSR	**L**anthanide **S**hift **R**eagent
LUT	**L**ook**U**p **T**able
MAGROFI	**MA**gnetization **G**rid **RO**tating-**F**rame **I**maging
MARCO POLO	**M**ultiple **A**nalysis by **R**eduction of **C**ross peaks and **O**rdering of **P**atterns in an **O**verdetermined **L**ibrary **O**rganization
MARDI-GRAS	**M**atrix **A**nalysis of **R**elaxati-on for **DI**stance **G**eomet**R**y of an **A**queous **S**tructure
MARF	**M**agic **A**ngle in the **R**otating **F**rame
MAS	**M**agic-**A**ngle **S**pinning
MASS	**M**agic-**A**ngle **S**ample **S**pinning
MAST	**M**otion **A**rtifact **S**uppression **T**echnique
MDEFT	**M**odified **D**riven **E**quilibrium **FT** method
ME	**M**ulti**E**cho
MEDUSA	Technique for the Determination of Dynamic Structures
MEM	**M**aximum **E**ntropy **M**ethod
MEMP	**M**ulti**E**cho **M**ulti**P**lanar
MESS	**M**ulti**E**cho **S**ingle **S**hot
MFISP	**M**irrored **FISP** (PSIF)
MGE	**M**ultiple **G**radient **E**cho
MININP	**MIN**inmum **I**ntensity **P**rojection
MIP	**M**aximum **I**ntensity **P**rojection
MLEV	M. Levitt's CPD sequence
MLM	**M**aximum **L**ikelihood **M**ethod
MOTSA	**M**ultiple **O**verlapping **T**hin **S**lab(Slice) **A**cquisition
MP	**M**ultiple **P**ulse, **M**ulti**P**lanar, **M**agnetization-**P**repared
MPF*n*	**M**ultiple-**P**ulse Decoupling with **P**hase and **F**requency Switching with ***n*** offsets
MP-GR	**M**ulti**P**lanar **G**radient-**R**e-called Acq. in Steady State
MPR	**M**ulti**P**lanar **R**econstruction
MP-RAGE	**M**agnetization-**P**repared **RA**pid **G**radient **E**cho (MP-GRE)
MQ	**M**ultiple-**Q**uantum
MQC	**M**ultiple-**Q**uantum **C**oherence
MQF	**M**ultiple-**Q**uantum **F**ilter
MQHPT	**M**ultiple-**Q**uantum **H**eteronuclear **P**olarization **T**ransfer
MQS	**M**ultiple-**Q**uantum **S**pectroscopy
MR	**M**agnetic **R**esonance
MRA	**MR A**ngiography
MREV-*n*	**M**ansfield-**R**him-**E**lleman-**V**aughan homonuc. dipolar dec. cycle of ***n*** pulses
MRV	**MR V**enography
MRI	**M**agnetic **R**esonance **I**maging
MRS	**M**agnetic **R**esonance **S**pectroscopy
MRSI	**M**agnetic **R**esonance **S**pectroscopic **I**maging
MRT	**M**agnetic **R**esonance **T**omography
MS	**M**ulti**S**lice
mSENSE	**m**odified **SENSE**
MS-EPI	**M**ulti**S**hot **EPI**
MSHOT-*n*	**M**agic **S**andwich **H**igh-**O**rder **T**runcation homo-nuc. dipolar decoupling sequence with ***n*** TREV-4 sandwiches
MSME	**M**ulti**S**lice **M**ulti**E**cho (T2 mapping)
MSOFT	**M**ulti**S**lice **O**ff-resonance **FaT** Suppression
MSP	**M**ultiple **S**ensitive **P**oint
MSPGSE	**M**ultiple-**S**tepped **PGSE**
MT	**M**agnetization **T**ransfer
MTC	**M**agnetization **T**ransfer **C**ontrast
MTSA	**M**ultiple **T**hin-**S**lab **A**cquisition
MUSIC	**MU**ltiplicity-**S**elective **I**n-phase **C**oherence transfer
MVS	**M**ultiple **V**olume **S**pectroscopy
NEDOR	**N**uclear **E**lectronic **DO**uble **R**esonance
NERO	**N**onlinear **E**xcitation with **R**ejection on **R**esonance
NEWS	**N**arrow-gap non-**E**xcitation for **W**ater **S**uppression
NEX	**N**umber of **EX**citations
NMR	**N**uclear **M**agnetic **R**esonance
NOE	**N**uclear **O**verhauser **E**ffect
NOE-DIFF	**NOE-DIFF**erence spectroscopy
NOESY	**NOE**-based 2D shift correlation
NOVEL	**N**uclear **O**rientation **V**ia **E**lectron spin **L**ocking
NPW	**N**o **P**hase **W**rap
NQCC	**N**uclear **Q**uadrupole **C**oupling **C**onstant
NQR	**N**uclear **Q**uadrupole **R**esonance
NQS	**N**on-**Q**uaternary **S**uppression
NSPECT	**N**on-localized **SPECT**roscopy
OBTUSE	**O**ffset **B**inomial **T**ailored for **U**niform **S**pectral **E**xcitation
OCS	**O**ptimized **C**osine-**S**ine pulse
ODMR	**O**ptically **D**etected **M**agnetic **R**esonance
OS	**O**vercontiguous **S**lices
OSIRIS	**O**uter-Volume-**S**uppressed **I**mage-**R**elated **I**n vivo **S**pectroscopy – a modifica-tion of ISIS
PACE	**P**rospective **A**cquisition **C**orr**E**ction
PAR	**P**hase-**A**lternated **R**otation of magnetization

Abbreviations and Acronyms Used in Magnetic Resonance

PARACEST	**PARA**magnetic **C**hemical **E**xchange **S**aturation **T**ransfer
PAS	**P**rincipal **A**xis **S**ystem
PC	**P**hase **C**ontrast
PCA	**P**hase **C**ontrast **A**ngio-graphy
P.COSY	**P**urged **COSY**
PD	**P**roton **D**ensity
PDLF	**P**roton-**D**etected **L**ocal **F**ield
PE	**P**hase **E**ncoding
P.E.COSY	**P**rimitive **E.COSY**, **P**urged **E**xclusive **COSY**
PEDRI	**P**roton-**E**lectron **D**ouble **R**esonance **I**maging
PELF	**P**roton-**E**ncoded **L**ocal **F**ield
PENDANT	**P**olarization **EN**hancement **D**uring **A**ttached **N**ucleus **T**esting
PEP	**P**reservation of **E**quivalent **P**athways
PFG	**P**ulsed **F**ield **G**radient
PFGSE	**P**ulsed **F**ield **G**radient **S**pin **E**cho
PGSE	**P**ulsed **G**radient **S**pin **E**cho
PISEMA	**P**olarization **I**nversion with **S**pin **E**xchange at the **M**agic **A**ngle
PITANSEMA	**P**olarization **I**nversion **T**ime **A**veraged **N**utation **S**pin **E**xchange at the **M**agic **A**ngle
PJR	**P**ower-adapted **J**ump and **R**eturn
PMFG	**P**ulsed **M**agnetic **F**ield **G**radient
PMLG	**P**hase-**M**odulated **L**ee-**G**oldburg dipolar decoupling
PMRFI	**P**hase-**M**odulated **R**otating-**F**rame **I**maging
POF	**P**roduct **O**perator **F**ormalism
POMMIE	**P**hase **O**scillations to **M**axi**MI**ze **E**diting
POST	**P**ermutationally **O**ffset-**ST**abilized
PRE	**P**roton **R**elaxation **E**nhancement
Presat	**Presat**uration (usually of solvent)
PRESS	**P**oint-**RES**olved **S**pectroscopy
PRFT	**P**artially **R**elaxed **F**ourier **T**ransform
PROPELLER	**P**eriodically **R**otated **O**ver-lapping **P**aral**lEL** **L**ines with **E**nhanced **R**econstruction
PS	**P**artial **S**aturation
PS-COSY	**P**hase-**S**ensitive **COSY**
PSD	**P**hase-**S**ensitive **D**etection
PSIF	mirrored **FISP** (SE acquisition)
PT	**P**olarization **T**ransfer
PW	**P**ulse **W**idth
PWI	**P**erfusion-**W**eighted **I**maging
Q	**Q**uality **F**actor (of RF coil/circuit) **Q**uantitative … (e.g. **QMRI**, **QCSI**)
Q.F	**Q**uadrupole moment/**F**ield gradient (interaction or relaxation mechanism)
Q Flow	**Flow Q**uantification
QPD	**Q**uadrature **P**hase **D**etection
QUEST	**QU**ick **E**cho **S**plit Imaging **T**echnique
QUIPSS	**QU**antitative **I**maging of **P**erfusion using a **S**ingle **S**ubtraction
RAM	**R**apid **A**cquisition **M**atrix
RARE	**R**apid **A**cquisition **R**elaxation **E**nhanced
RAREst	**RARE** with **s**hort **t**E using slew-rate-optimized gradients
RAREVTR	**RARE** with **V**ariable **TR** (simultaneous T_1 & T_2 mapping)
RASE	**R**apid **A**cquisition **S**pin **E**cho
RBW	**R**eceiver **B**and**W**idth
RCF	**R**otating **C**oordinate **F**rame
RCT	**R**elayed **C**oherence **T**ransfer
RE	**R**apid **E**xcitation (MRI)
REAPDOR	**R**otational **E**cho **A**diabatic **P**assage **DO**uble **R**esonance
RE-BURP	**Re**focused **B**and-selective **U**niform **R**esponse **P**ure phase
RECSY	Multistep **RE**layed **C**oherence **S**pectroscop**Y**
REDOR	**R**otational **E**cho **DO**uble **R**esonance
RELAY	**RELAY**ed Correlation Spectroscopy
REPAY	**R**everse **E**diting of **P**rotons **A**ccording to multiplicit**Y**
REREDOR	**R**otor-**E**ncoded **REDOR**
REST	**RE**gional **S**aturation **T**echnique
RF	**R**adio **F**requency
RFDR	**RF-D**riven **R**ecoupling
RF-FAST	**RF**-spoiled **FAST**
RFOV	**R**ectangular **FOV**
RICE	**R**apid **I**maging using **C**om-posite **E**cho
RIDE	**RI**ng **D**own **E**limination
RINEPT	**R**everse **INEPT**
RISE	**R**apid **I**maging using **S**pin **E**cho
RMSD	**R**oot-**M**ean-**S**quare **D**eviation
ROAST	**R**esonant **O**ffset **A**veraging in the **ST**eady State
RODI	**RO**tatin-grame relaxation **D**ispersion **I**maging
ROE	**R**otating-frame **O**verhauser **E**ffect
ROESY	**ROE**-based 2D shift correlation
ROI	**R**egion **O**f **I**nterest
ROPE	**R**espiratory **O**rdered **PE**
ROTO	**RO**ESY-**TO**CSY Relay
RPA	**R**andom **P**hase **A**pproximation
RR	**R**otational **R**esonance
RSSARGE	**R**F-**S**poiled **SARGE**
RT	**R**espiratory **T**rigger
RUFIS	**R**otating **U**ltra**F**ast **I**maging **S**equence
SA	**S**hielding **A**nisotropy
SAR	**S**pecific **A**bsorption **R**ate (RF)
SARGE	**S**poiled steady-state **A**cquisition with **R**ewinded **G**radient **E**cho
SAT	**SAT**uration
SB	**S**ine-**B**ell window function
SC	**S**calar **C**oupling
S.COSY	**COSY** with shift **S**caling in F1
SCT	**SC**an **T**ime
SCUBA	**S**timulate **C**ross peaks **U**nder **B**leached **A**lphas
SD	**S**pin **D**ipolar

Abbreviations and Acronyms Used in Magnetic Resonance

SDDS	**S**pin **D**ecoupling **D**ifference **S**pectroscopy
SDEPT	**S**elective **DEPT**
SE	**S**pin **E**cho
SECSY	**S**pin-**E**cho **C**orrelated Spectroscop**Y**
SEDOR	**S**pin-**E**cho **DO**uble **R**esonance
SEDRA	**S**imple **E**xcitation for **D**ephasing of **R**otational echo **A**mplitudes
SEDUCE	**SE**lective **D**ecoupling **U**sing **C**rafted **E**xcitation
SEFT	**S**pin-**E**cho **F**ourier **T**ransform Spectroscopy (with J modulation)
SELCOSY	**SEL**ective **COSY**
SELTICS	**S**ideband **EL**imination by **T**emporary **I**nterruption of the **C**hemical **S**hift
SELINCOR	**SEL**ective **IN**verse **COR**relation
SELINQUATE	**SEL**ective **IN**ADE**QUATE**
SELRESOLV	**SEL**ective **RES**olution of C,H Coupling
SEMS	**S**pin-**E**cho **M**ulti**S**lice
SEMUT	**S**ubspectral **E**diting Using a **MU**ltiple-Quantum **T**rap
SENSE	**SENS**itivity **E**ncoding
sEPI	**s**piral **EPI**
SEPT	**S**elective IN**EPT**
SERF	**SE**lective **R**e**F**ocussing
SESAM	**SE**mi-**S**elective **A**cquisition **M**odulated (Decoupling)
SFAM	**S**imultaneous **F**req. and **A**mpl. **M**odulation
SFORD	**S**ingle **F**requency **O**ff-**R**esonance **D**ecoupling
SGSE	**S**teady-**G**radient **S**pin-**E**cho
SHECOR	**S**elective **HE**teronuclear **COR**relation
SHORT	**SHORT** repetition techniques
SI	**S**pectroscopic **I**maging
SIAM	**Si**multaneous acq. of **I**n-phase and **A**ntiphase **M**ultiplets
SIP	**S**aturation **I**nversion **P**rojection
SIMBA	**S**elective **I**nverse **M**ultiple-**B**ond **A**nalysis
SINEPT	**SINE**-dependent **PT**
SINGLE PULSE	**SINGLE PULSE**-acquire spectroscopy
SIS	**S**ubstituent-**I**nduced **S**hift
SJR	**S**econd-order **J**ump and **R**eturn
SKEWSY	**SKEW**ed Exchange Spectroscop**Y**
SL	**S**pin-**L**ock pulse
SLF	**S**eparated **L**ocal **F**ield
SLITDRESS	**SLI**ce in**T**erleaved **D**epth **RE**solved **S**urface coil **S**pectroscopy
SLOPT	**S**pin-**LO**cking **P**olarization **T**ransfer
SMART	**S**himadzu **M**otion **A**rtifact **R**eduction **T**echnique
SMASH	**S**hort **M**inimum **A**ngle **SH**ot, **SiM**ultaneous **A**cquisition of **S**patial **H**armonics
SNR or S/N	**S**ignal-to-**N**oise **R**atio
SOPPA	**S**econd-**O**rder **P**olarization **P**ropagator **A**pproach
SORS/STC	**S**lice-selective **O**ff-**R**esonance **S**inc Pulse **/ S**aturation **T**ransfer **C**ontrast
SPACE	**SPA**tial and **C**hemical-Shift Encoded **E**xcitation
SPAIR	**SP**ectral Selection **A**ttenuated **I**nversion **R**ecovery
SPECIFIC-CP	**SPEC**trally **I**nduced **F**iltering **I**n **C**ombination with **C**ross **P**olarization
SPEED	**S**wap **P**has**E**-**E**ncoded **D**ata
SPGR	**SP**oiled **G**radient-**R**ecalled
SPI	**S**elective **P**opulation **I**nversion
SPIDER	**S**teady-state **P**rojection **I**maging with **D**ynamic **E**cho **T**rain **R**eadout
SPIO	**S**uper**P**aramagnetic **I**ron **O**xide
SPIR	**S**pectral **P**resaturation **I**nversion-**R**ecovery
SPIRAL	MRI with **SPIRAL** *k*-space scan
SPRITE	**S**ingle-**P**oint **R**amped **I**maging with **T**1 **E**nhancement
SPT	**S**elective **P**opulation **T**ransfer
SQ	**S**ingle-**Q**uantum
SQC	**S**ingle-**Q**uantum **C**oherence
SQF	**S**ingle-**Q**uantum **F**ilter
SR	**S**aturation-**R**ecovery
SRP	**S**elf-**R**efocusing **P**ulse
SS	**S**lice **S**election (gradient), **S**ingle **S**lice
SSB	**S**hifted **S**ine-**B**ell window function
SSFP	**S**teady-**S**tate **F**ree **P**recession
SSFSE	**S**ingle-**S**hot **FSE**
SSI	**S**olid **S**tate **I**maging
SSMP	**S**ingle-**S**lice **M**ultiple-**P**hase
ssNMR	**s**olid-**s**tate **NMR**
SSTSE/T2	**S**ingle-**S**hot **TSE** with **T2** weighting
ST	**S**aturation **T**ransfer, **S**lice **T**hickness
STAGE	**S**mall **T**ip **A**ngle **GE**
STE	**ST**imulated **E**cho
STEAM	**ST**imulated **E**cho **A**cquisition **M**ode for imaging
STEP	**STE P**rogressive Imaging
STERF	**S**teady-State **TE**chnique with **R**efocused **F**ID
STIR	**S**hort **T**1 **I**nversion-**R**ecovery
STREAM	**S**uppressed **T**issue with **RE**freshment **A**ngiography **M**ethod
STUD	**S**ech/**T**anh **U**niversal **D**ecoupling – an adiabatic decoupling scheme
SUBMERGE	**SU**ppression **B**y **M**istuned **E**cho and **R**epetitive **G**radient **E**pisodes
SUSAN	**S**pin decoupling employing **U**ltra-broadband inversion sequences generated via **S**imulated **AN**nealing
SWATTR	**S**elective **W**ater **A**ttenuation by **T2** and **T1** **R**elaxation
SVS	**S**ingle-**V**olume **S**pectroscopy
T1 ...	**T1**-weighted ... (method)
T1W	**T1-W**eighted
T2 ...	**T2**-weighted ... (method)
T2W	**T2-W**eighted
T2*W	**T2*-W**eighted
TACSY	**TA**ylored **C**orrelation Spectroscop**Y**
TANGO	**T**esting for **A**djacent **N**uclei with a **G**yration **O**perator

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

TART	**T**ip **A**ngle **R**educed T_1 Imaging
TD	**T**rigger **D**elay, **T**ime **D**ifference
TCF	**T**ime **C**orrelation **F**unction
TE	**T**ime delay between excitation and **E**cho maximum
TEDOR	**T**ransferred-**E**cho **DO**uble **R**esonance
TEI	**TE** **I**nterleaved
TF	**T**urbo **F**actor
TFE	**T**urbo **F**ield **E**cho
TGSE	**T**urbo **G**radient **S**pin **E**cho
THRIVE	**T**1W **H**igh-**R**esolution **I**sotropic **V**olume **E**xamination
TI	**T**ime following **I**nversion
TIR	**T**urbo **IR**
TMR	**T**opical **M**agnetic **R**esonance
TOBSY	**TO**tal through-**B**ond correlation **S**pectroscop**Y**
TOCSY	**TO**tal **C**orrelation **S**pectroscop**Y**
TOF	**T**ime-**O**f-**F**light
TOE	**T**runcated N**OE**
TONE	**T**ilt-**O**ptimized **N**onsaturated **E**xcitation
TORO	**TO**CSY-**RO**ESY Relay
TOSS	**TO**tal **S**uppression of **S**idebands
TPPI	**T**ime-**P**roportional **P**hase **I**ncrementation
TPPM	**T**wo-**P**ulse **P**hase **M**odulation
TPR	**T**ime and **P**hase **R**eversal
TQ	**T**riple-**Q**uantum
TQF	**T**riple-**Q**uantum **F**ilter
TR	**T**ime for **R**epetition of excitation
T/R	**T**ransmit/**R**eceive
TRAPDOR	**TRA**nsfer of **P**opulations in **DO**uble **R**esonance
TRCF	**T**ilted **R**otating **C**oordinate **F**rame
TREV-*n*	**T**ime-**REV**ersal echo sequence of ***n*** pulses for homonuc. dipolar dec.
TRNOE	**TR**ansferred **NOE**
TROSY	**T**ransverse **R**elaxation **O**ptimized **S**pectroscop**Y**
T-ROESY	**T**ransverse **ROESY**

TrueFISP	**FISP** with balanced gradient waveform
TS	**T**ime of **S**aturation
TSE	**T**urbo **S**pin **E**cho
TSETSE	double-resonance **T**wo-**S**pin **E**ffect for correlation spectroscopy
TSR	**T**otal **SR**
Turbo-FLASH	**FLASH** sequence during one IR period
U-BURP	**U**niversal **BURP** pulse
UE	**U**npaired **E**lectron (relaxation mechanism)
UFSE	**U**ltra**F**ast **SE**
UNCOSY	**UN**iform excitation **COSY**
USPIO	**U**ltra**S**mall **P**aramagnetic **I**ron **O**xide
UTE	**U**ltra-short **TE** radial scan
UTSE	**U**ltra-short **TSE**
VAPRO	**VA**riable **PRO**jection method
VAS	**V**ariable **A**ngle **S**pinning
VE	**V**elocity-**E**ncoded
VEC	**V**elocity-**E**ncoded **C**ine (MRI)
VEMP	**V**ariable-**E**cho **M**ulti**P**lanar
VENC	**V**elocity **ENC**oding value
VEST	**V**olume **E**xcitation **ST**imulated echoes
VIGRE	**V**olumetric **I**nterpolated **GR**adient **E**cho
VOI	**V**olume **O**f **I**nterest
VOSING	**VO**lume-selective **S**pectral edit**ING**
VOSY	**VO**lume-Selective **S**pectroscop**Y**
VPS	**V**olumes **P**er **S**egment
VSOP	**V**ery **S**mall superparamagnetic iron **O**xide **P**articles
WAHUHA	**WA**ugh-**HU**ber-**HA**eberlen Sequence
WALTZ	CPD Sequence Containing the Elements 1-2-3
WATER-GATE	**WATER** suppression through **GrA**dient **T**ailored **E**xcitation
WATR	**W**ater **A**ttenuation by **T**ransverse **R**elaxation
WEFT	**W**ater **E**liminated **F**ourier **T**ransform
WET	**W**ater suppression **E**nhanced through **T**1 effects

WFOP	**W**ater **F**at **O**pposed **P**hase
WFS	**W**ater **F**at **S**eparation (Shift Difference)
WHH-*n*	**WAHUHA** dec. cycle of ***n*** pulses
WIM-*n*	**W**indowless **I**sotropic **M**ixing dec. cycle of ***n*** pulses
WURST	**W**ideband, **U**niform **R**ate, and **S**mooth **T**runcation – an adiabatic decoupling sequence
XCORFE	H, **X** **COR**relation using a **F**ixed **E**volution time
XD-NOESY	e**X**change-**D**ecoupled **NOESY**
X-FILTER	Selection of ^{1}H-^{1}H correlation when both H are coupled to X
X-HALF-FILTER	Selection of ^{1}H-^{1}H correlation when one H is coupled to X
Z-COSY	**Z**-filtered **COSY**
Z-FILTER	pulse sandwich for elimination of signal components with dispersive phase
ZECSY	**Z**ero-Quantum-**E**cho **C**orrelation **S**pectroscop**Y**
ZIP	**Z**ero-fill **I**nterpolation **P**rocessing
ZQ	**Z**ero **Q**uantum
ZQC	**Z**ero-**Q**uantum **C**oherence
ZQF	**Z**ero-**Q**uantum **F**ilter
ZZ-Spectroscopy	Selection of coherences involving ZZ or longitudinal two-spin order
ZZZ-Spectroscopy	Selection of coherences involving longitudinal 3-spin order
β-COSY	COSY with low-angle mixing pulse
Ψ-COSY	pseudo-COSY using incremented freq.-selective excitation

Symbols for NMR and Related Quantities*

Roman alphabet	
a or A	Hyperfine (electron-nucleus) coupling constant
$A_q^{(l,m)}$	The mth component of an irreducible tensor of order l representing the nuclear spin operator for an interaction of type q
$\boldsymbol{B}$	Magnetic field (strictly the magnetic flux density or magnetic induction)
$\boldsymbol{B}_0$	Static magnetic field of an NMR spectrometer
$\boldsymbol{B}_1$, $\boldsymbol{B}_2$	Radiofrequency magnetic fields associated with frequencies ν_1, ν_2
$\boldsymbol{B}_L$	Local magnetic field of random field or dipolar origin
$\boldsymbol{C}$	Spin-rotation interaction tensor
C_X	Spin-rotation coupling constant of nuclide X
$\boldsymbol{D}$	Dipolar interaction tensor
$D_{i,j}$	Dipolar coupling constant between nuclei (i and j), in Hz
D^C	Nuclear receptivity relative to that of ^{13}C
D^P	Nuclear receptivity relative to that of ^{1}H
$\boldsymbol{E}$	Electric field strength
F	Spectral width
F_1, F_2 or f_1, f_2	The two frequency dimensions of a two-dimensional spectrum
$\hat{\boldsymbol{F}}_G$	Nuclear spin operator for a group, G, of nuclei
F_G	Magnetic quantum number associated with $\hat{\boldsymbol{F}}_G$
g	Nuclear or electronic g factor (Landé splitting factor)
G	Magnetic field gradient amplitude
$\hat{\boldsymbol{H}}$	Hamiltonian operator
$H_{i,j}$	Matrix element of Hamiltonian operator
$\hat{\boldsymbol{I}}_j$	Nuclear spin operator for nucleus j
$\hat{I}_{j+}$, $\hat{I}_{j-}$	'Raising' and 'lowering' spin operators for nucleus j
I_j	Magnetidc quantum number associated with $\hat{\boldsymbol{I}}_j$
$\boldsymbol{J}$	Indirect coupling tensor
$^nJ_{AB}$	Spin-spin coupling constant for nuclei A and B through n bonds in Hz
$J(\omega)$	Spectral density of fluctuations at angular frequency ω
$^nK_{AB}$	Reduced nuclear spin-spin coupling constant $K_{AB} = 4\pi^2 J_{AB}/h\gamma_A\gamma_B)$ in T^2J^{-1}

$\boldsymbol{L}$	Angular momentum
m_j	Eigenvalue of $\hat{\boldsymbol{I}}_{jz}$ (magnetic component quantum number)
m_{tot}	Total magnetic component quantum number for a spin system (eigenvalue of $\sum_j \hat{\boldsymbol{I}}_{jz}$)
$m_{tot}(X)$	Total magnetic component quantum number for X-type nuclei
$\boldsymbol{M}_0$	Equilibrium macroscopic magnetization per unit volume in the presence of $\boldsymbol{B}_0$
M_x, M_y, M_z	Components of macroscopic magnetization per volume
M_n	nth moment of spectrum (M_2 = second moment, etc.)
n_α, n_β	Populations of the α and β spin states
N	Total number of nuclei of a given type per unit volume in the sample
$\boldsymbol{q}$	Electric field gradient tensor in units of the elementary charge
eQ	Nuclear quadrupole moment, Q is in m^2 and e is the elementary charge in C
R_1^X	Spin-lattice (longitudinal) relaxation rate constant for nucleus X
R_2^X	Spin-spin (transverse) relaxation rate constant for nucleus X
$R_{1\rho}^X$	Longitudinal relaxation rate constant for nucleus X in the reference frame rotating with $\boldsymbol{B}_1$
S	Signal intensity
$\hat{\boldsymbol{S}}$	Electron (or, occasionally, nuclear) spin operator; cf. $\hat{\boldsymbol{I}}$
t_1, t_2	Time dimensions for two-dimensional NMR
T_c	Coalescence temperature under chem. exchange for signals in an NMR spectrum
T_1^X	Spin-lattice (longitudinal) relaxation time of the X nucleus
T_2^X	Spin-spin (transverse) relaxation time of the X nucleus
T_2^*	Net dephasing time for M_x or M_y
$T_{1\rho}^X$	Longitudinal relaxation time for the X nucleus in the reference frame rotating with $\boldsymbol{B}_1$
T_d	Pulse (recycle) delay
T_{ac}	Acquisition time
$T_q^{(l,m)}$	The mth component of an irreducible tensor of order l representing the strength of an interaction of type q

** IUPAC Recommendations: Magnetic Resonance in Chemistry, Vol. 36, 145-149 (1998)*

NMR Tables

Symbols for NMR and Related Quantities*

$\boldsymbol{V}$	Electric field gradient tensor. $\boldsymbol{V} = e\boldsymbol{q}$, where e is the elementary charge
$V_{\alpha\beta}$	Elements of Cartesian electric field gradient tensor
W_0, W_1, W_2	Relaxation rate constants (transition probabilities per time) between energy levels differing by 0, 1 and 2 in m_{tot}
W_{rs}	Transition probability between spin states r and s
Greek alphabet	
α	Nuclear spin wavefunction (eigenfunction of $\hat{I}_z$) for the $m_I = +\frac{1}{2}$ state of a spin-½ nucleus
α_E	The Ernst angle (for optimum sensitivity)
β	Nuclear spin wavefunction (eigenfunction of $\hat{I}_z$) for the $m_I = -\frac{1}{2}$ state of a spin-½ nucleus
γ_X	Magnetogyric ratio of nucleus X
δ_X	Chemical shift (for the resonance) of nucleus of element X, usually in ppm
Δn	Population difference between nuclear states (Δn_0 at Boltzmann equilibrium)
$\Delta\delta$	Change or difference in δ
$\Delta\nu_{1/2}$	Full width in frequency units of a resonance line at half-height
$\Delta\sigma$	Anisotropy in σ [$\Delta\sigma = \sigma_{zz} - \frac{1}{2}(\sigma_{xx} + \sigma_{YY})$]
$\Delta\chi$	(i) Susceptibility anisotropy ($\Delta\chi = \chi_{\parallel} - \chi_{\perp}$); (ii) difference in electronegativities
ε_0	Permittivity of the vacuum
ζ	Anisotropy in shielding, expressed as $\sigma_{zz} - \sigma_{iso}$
η	(i) Nuclear Overhauser enhancement; (ii) tensor asymmetry factor; (iii) viscosity
κ	Skew of a tensor
θ	Angle, especially for that between a given vector and $\boldsymbol{B}_0$
$\boldsymbol{\mu}$	(i) Magnetic dipole moment (component μ_z along $\boldsymbol{B}_0$); (ii) electric dipole moment
μ_0	Permeability of the vacuum
μ_B	Bohr magneton (earlier β_e)
μ_N	Nuclear magneton (earlier β_N)
ν_j	Larmor or resonance frequency of nucleus j (in Hz)
ν_0	(i) Spectrometer operating frequency; (ii) Basic Larmor or resonance frequency for a given isotope

ν_1	Frequency of primary RF magnetic field B_1 (excitation, detection)
ν_2	Frequency of secondary RF magnetic field B_2 (decoupling)
Ξ_X	Normalized resonance frequency for nucleus X relative to ν_H for tetramethylsilane (TMS) at the same $\boldsymbol{B}_0$ field; $\Xi_x = 100\ \nu_x/\nu_H$ (TMS)
ρ	Density matrix
$\hat{\rho}$	Density operator
ρ_{ij}	Element of matrix representation of $\hat{\rho}$
$\boldsymbol{\sigma}$	Shielding tensor
σ_j	(Isotropic) shielding constant of nucleus j
$\sigma_{\parallel}$, $\sigma_{\perp}$	Components of shielding tensor σ parallel and perpendicular to the symmetry axis
$\hat{\sigma}$	Reduced density operator
τ	(i) Time between RF pulses or recovery time following inversion (ii) lifetime in dynamic NMR studies
τ_c	Correlation time for molecular motion, especially for isotropic molecular tumbling
τ_d	Dwell time for data sampling
τ_{null}	Recovery time leading to null M_z after a 180° pulse
τ_p	Pulse duration
τ_{sc}	Correlation time for relaxation by the scalar mechanism
τ_{sr}	Correlation time for spin-rotation relaxation
$\tau_{\parallel}$, $\tau_{\perp}$	Correlation times for molecular tumbling parallel and perpendicular to the symmetry axis
χ	(i) Magnetic susceptibility; (ii) nuclear quadrupole coupling constant ($\chi = e^2 q_{ZZ} Q/h$)
$\omega_j, \omega_0, \omega_1, \omega_2$	As for ν_j, ν_0, ν_1, ν_2 but in angular frequency units (rad/s)
Ω	Span of a tensor
Ω_1, Ω_2	Angular frequency of RF fields $\boldsymbol{B}_1$, $\boldsymbol{B}_2$

* IUPAC Recommendations: Magnetic Resonance in Chemistry, Vol. 36, 145-149 (1998)

NMR Tables

BRUKER

^{1}H Chemical Shifts for Common Contaminants in Deuterated Solvents

	Proton	mult., J	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
residual solvent H			7.26	2.05	2.50	7.16	1.94	3.31	4.79
H_2O		s	1.56	2.84 [a]	3.33 [a]	0.40	2.13	4.87	
acetic acid	CH_3	s	2.10	1.96	1.91	1.55	1.96	1.99	2.08
acetone	CH_3	s	2.17	2.09	2.09	1.55	2.08	2.15	2.22
acetonitrile	CH_3	s	2.10	2.05	2.07	1.55	1.96	2.03	2.06
benzene	CH	s	7.36	7.36	7.37	7.15	7.37	7.33	
t-butanol	CH_3	s	1.28	1.18	1.11	1.05	1.16	1.40	1.24
	OH [c]	s			4.19	1.55	2.18		
t-butyl methyl ether	CCH_3	s	1.19	1.13	1.11	1.07	1.14	1.15	1.21
	OCH_3	s	3.22	3.13	3.08	3.04	3.13	3.20	3.22
BHT [b]	ArH	s	6.98	6.96	6.87	7.05	6.97	6.92	
	OH [c]	s	5.01		6.65	4.79	5.20		
	$ArCH_3$	s	2.27	2.22	2.18	2.24	2.22	2.21	
	$ArC(CH_3)_3$	s	1.43	1.41	1.36	1.38	1.39	1.40	
chloroform	CH	s	7.26	8.02	8.32	6.15	7.58	7.90	
cyclohexane	CH_2	s	1.43	1.43	1.40	1.40	1.44	1.45	
1,2-dichloroethane	CH_2	s	3.73	3.87	3.90	2.90	3.81	3.78	
dichloromethane	CH_2	s	5.30	5.63	5.76	4.27	5.44	5.49	
diethyl ether	CH_3	t, 7	1.21	1.11	1.09	1.11	1.12	1.18	1.17
	CH_2	q, 7	3.48	3.41	3.38	3.26	3.42	3.49	3.56
diglyme	CH_2	m	3.65	3.56	3.51	3.46	3.53	3.61	3.67
	CH_2	m	3.57	3.47	3.38	3.34	3.45	3.58	3.61
	OCH_3	s	3.39	3.28	3.24	3.11	3.29	3.35	3.37
1,2-dimethoxyethane	CH_3	s	3.40	3.28	3.24	3.12	3.28	3.35	3.37
	CH_2	s	3.55	3.46	3.43	3.33	3.45	3.52	3.60
dimethylacetamide	CH_3CO	s	2.09	1.97	1.96	1.60	1.97	2.07	2.08
	NCH_3	s	3.02	3.00	2.94	2.57	2.96	3.31	3.06
	NCH_3	s	2.94	2.83	2.78	2.05	2.83	2.92	2.90
dimethylformamide	CH	s	8.02	7.96	7.95	7.63	7.92	7.97	7.92
	CH_3	s	2.96	2.94	2.89	2.36	2.89	2.99	3.01
	CH_3	s	2.88	2.78	2.73	1.86	2.77	2.86	2.85
dimethylsulfoxide	CH_3	s	2.62	2.52	2.54	1.68	2.50	2.65	2.71
dioxane	CH_2	s	3.71	3.59	3.57	3.35	3.60	3.66	3.75
ethanol	CH_3	t, 7	1.25	1.12	1.06	0.96	1.12	1.19	1.17
	CH_2	q, 7 [d]	3.72	3.57	3.44	3.34	3.54	3.60	3.65
	OH	s [c,d]	1.32	3.39	4.63		2.47		
ethyl acetate	CH_3CO	s	2.05	1.97	1.99	1.65	1.97	2.01	2.07
	CH_2CH_3	q, 7	4.12	4.05	4.03	3.89	4.06	4.09	4.14
	CH_2CH_3	t, 7	1.26	1.20	1.17	0.92	1.20	1.24	1.24
ethyl methyl ketone	CH_3CO	s	2.14	2.07	2.07	1.58	2.06	2.12	2.19
	CH_2CH_3	q, 7	2.46	2.45	2.43	1.81	2.43	2.50	3.18
	CH_2CH_3	t, 7	1.06	0.96	0.91	0.85	0.96	1.01	1.26
ethylene glycol	CH	s [e]	3.76	3.28	3.34	3.41	3.51	3.59	3.65
"grease" [f]	CH_3	m	0.86	0.87		0.92	0.86	0.88	
	CH_2	br s	1.26	1.29		1.36	1.27	1.29	
n-hexane	CH_3	t	0.88	0.88	0.86	0.89	0.89	0.90	
	CH_2	m	1.26	1.28	1.25	1.24	1.28	1.29	
HMPA [g]	CH_3	d, 9.5	2.65	2.59	2.53	2.40	2.57	2.64	2.61
methanol	CH_3	s [h]	3.49	3.31	3.16	3.07	3.28	3.34	3.34
	OH	s [c,h]	1.09	3.12	4.01		2.16		
nitromethane	CH_3	s	4.33	4.43	4.42	2.94	4.31	4.34	4.40
n-pentane	CH_3	t, 7	0.88	0.88	0.86	0.87	0.89	0.90	
	CH_2	m	1.27	1.27	1.27	1.23	1.29	1.29	

*Reprinted with permission from: J. Org. Chem. 1997, **62**, 7512-7515*

© 1997 American Chemical Society

^{1}H Chemical Shifts for Common Contaminants in Deuterated Solvents (continued)

	Proton	mult.	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
i-propanol	CH_3	d, 6	1.22	1.10	1.04	0.95	1.09	1.50	1.17
	CH	sep, 6	4.04	3.90	3.78	3.67	3.87	3.92	4.02
pyridine	CH(2)	m	8.62	8.58	8.58	8.53	8.57	8.53	8.52
	CH(3)	m	7.29	7.35	7.39	6.66	7.33	7.44	7.45
	CH(4)	m	7.68	7.76	7.79	6.98	7.73	7.85	7.87
silicone grease[i]	CH_3	s	0.07	0.13		0.29	0.08	0.10	
tetrahydrofuran	CH_2	m	1.85	1.79	1.76	1.40	1.80	1.87	1.88
	CH_2O	m	3.76	3.63	3.60	3.57	3.64	3.71	3.74
toluene	CH_3	s	2.36	2.32	2.30	2.11	2.33	2.32	
	CH(*o/p*)	m	7.17	7.1-7.2	7.18	7.02	7.1-7.3	7.16	
	CH(*m*)	m	7.25	7.1-7.2	7.25	7.13	7.1-7.3	7.16	
triethylamine	CH_3	t, 7	1.03	0.96	0.93	0.96	0.96	1.05	0.99
	CH_2	q, 7	2.53	2.45	2.43	2.40	2.45	2.58	2.57

[a] In these solvents the intermolecular rate of exchange is slow enough that a peak due to HDO is usually also observed; it appears at 2.81 and 3.30 ppm in acetone and DMSO, respectively. In the former solvent, it is often seen as a 1:1:1 triplet, with $^{2}J_{H,D}$ = 1 Hz. [b] 2,6-di-*tert*-butyl-4-methylphenol. [c] The signals from exchangeable protons were not always identified. [d] In some cases (see note *a*), the coupling interaction between the CH_2 and the OH protons may be observed (J = 5 Hz). [e] In CD_3CN, the OH proton was seen as a multiplet at δ = 2.69, and extra coupling was also apparent on the methylene peak. [f] Long-chain, linear aliphatic hydrocarbons. Their solubility in DMSO was too low to give visible peaks. [g] Hexamethylphosphoramide. [h] In some cases (see notes *a, d*), the coupling interaction between the CH_3 and the OH protons may be observed (J = 5.5 Hz). [i] Poly(dimethylsiloxane). Its solubility in DMSO was too low to give visible peaks.

^{13}C Chemical Shifts for Common Contaminants in Deuterated Solvents

		$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
solvent signals		77.16	29.84	39.52	128.06	1.32	49.00	
			206.26			118.26		
acetic acid	CO	175.99	172.31	171.93	175.82	173.21	175.11	177.21
	CH_3	20.81	20.51	20.95	20.37	20.73	20.56	21.03
acetone	CO	207.07	205.87	206.31	204.43	207.43	209.67	215.94
	CH_3	30.92	30.60	30.56	30.14	30.91	30.67	30.89
acetonitrile	CN	116.43	117.60	117.91	116.02	118.26	118.06	119.68
	CH_3	1.89	1.12	1.03	0.20	1.79	0.85	1.47
benzene	CH	128.37	129.15	128.30	128.62	129.32	129.34	
t-butanol	C	69.15	68.13	66.88	68.19	68.74	69.40	70.36
	CH_3	31.25	30.72	30.38	30.47	30.68	30.91	30.29
t-butyl methyl ether	OCH_3	49.45	49.35	48.70	49.19	49.52	49.66	49.37
	C	72.87	72.81	72.04	72.40	73.17	74.32	75.62
	CCH_3	26.99	27.24	26.79	27.09	27.28	27.22	26.60
BHT	C(1)	151.55	152.51	151.47	152.05	152.42	152.85	
	C(2)	135.87	138.19	139.12	136.08	138.13	139.09	
	CH(3)	125.55	129.05	127.97	128.52	129.61	129.49	
	C(4)	128.27	126.03	124.85	125.83	126.38	126.11	
	CH_3Ar	21.20	21.31	20.97	21.40	21.23	21.38	
	CH_3C	30.33	31.61	31.25	31.34	31.50	31.15	
	C	34.25	35.00	34.33	34.35	35.05	35.36	
chloroform	CH	77.36	79.19	79.16	77.79	79.17	79.44	
cyclohexane	CH_2	26.94	27.51	26.33	27.23	27.63	27.96	
1,2-dichloroethane	CH_2	43.50	45.25	45.02	43.59	45.54	45.11	
dichloromethane	CH_2	53.52	54.95	54.84	53.46	55.32	54.78	
diethyl ether	CH_3	15.20	15.78	15.12	15.46	15.63	15.46	14.77
	CH_2	65.91	66.12	62.05	65.94	66.32	66.88	66.42

^{13}C Chemical Shifts for Common Contaminants in Deuterated Solvents (continued)

		$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
diglyme	CH_3	59.01	58.77	57.98	58.66	58.90	59.06	58.67
	CH_2	70.51	71.03	69.54	70.87	70.99	71.33	70.05
	CH_2	71.90	72.63	71.25	72.35	72.63	72.92	71.63
1,2-dimethoxyethane	CH_3	59.08	58.45	58.01	58.68	58.89	59.06	58.67
	CH_2	71.84	72.47	17.07	72.21	72.47	72.72	71.49
dimethylacetamide	CH_3	21.53	21.51	21.29	21.16	21.76	21.32	21.09
	CO	171.07	170.61	169.54	169.95	171.31	173.32	174.57
	NCH_3	35.28	34.89	37.38	34.67	35.17	35.50	35.03
	NCH_3	38.13	37.92	34.42	37.03	38.26	38.43	38.76
dimethylformamide	CH	162.62	162.79	162.29	162.13	163.31	164.73	165.53
	CH_3	36.50	36.15	35.73	35.25	36.57	36.89	37.54
	CH_3	31.45	31.03	30.73	30.72	31.32	31.61	32.03
dimethyl sulfoxide	CH_3	40.76	41.23	40.45	40.03	41.31	40.45	39.39
dioxane	CH_2	67.14	67.60	66.36	67.16	67.72	68.11	67.19
ethanol	CH_3	18.41	18.89	18.51	18.72	18.80	18.40	17.47
	CH_2	58.28	57.72	56.07	57.86	57.96	58.26	58.05
ethyl acetate	CH_3CO	21.04	20.83	20.68	20.56	21.16	20.88	21.15
	CO	171.36	170.96	170.31	170.44	171.68	172.89	175.26
	CH_2	60.49	60.56	59.74	60.21	60.98	61.50	62.32
	CH_3	14.19	14.50	14.40	14.19	14.54	14.49	13.92
ethyl methyl ketone	CH_3CO	29.49	29.30	29.26	28.56	29.60	29.39	29.49
	CO	209.56	208.30	208.72	206.55	209.88	212.16	218.43
	CH_2CH_3	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	CH_2CH_3	7.86	8.03	7.61	7.91	8.14	8.09	7.87
ethylene glycol	CH_2	63.79	64.26	62.76	64.34	64.22	64.30	63.17
"grease"	CH_2	29.76	30.73	29.20	30.21	30.86	31.29	
n-hexane	CH_3	14.14	14.34	13.88	14.32	14.43	14.45	
	CH_2(2)	22.70	23.28	22.05	23.04	23.40	23.68	
	CH_2(3)	31.64	32.30	30.95	31.96	32.36	32.73	
HMPA[b]	CH_3	36.87	37.04	36.42	36.88	37.10	37.00	36.46
methanol	CH_3	50.41	49.77	48.59	49.97	49.90	49.86	49.50[c]
nitromethane	CH_3	62.50	63.21	63.28	61.16	63.66	63.08	63.22
n-pentane	CH_3	14.08	14.29	13.28	14.25	14.37	14.39	
	CH_2(2)	22.38	22.98	21.70	22.72	23.08	23.38	
	CH_2(3)	34.16	34.83	33.48	34.45	34.89	35.30	
i-propanol	CH_3	25.14	25.67	25.43	25.18	25.55	25.27	24.38
	CH	64.50	63.85	64.92	64.23	64.30	64.71	64.88
pyridine	CH(2)	149.90	150.67	149.58	150.27	150.76	150.07	149.18
	CH(3)	123.75	124.57	123.84	123.58	127.76	125.53	125.12
	CH(4)	135.96	136.56	136.05	135.28	136.89	138.35	138.27
silicone grease	CH_3	1.04	1.40		1.38		2.10	
tetrahydrofuran	CH_2	25.62	26.15	25.14	25.72	26.27	26.48	25.67
	CH_2O	67.97	68.07	67.03	67.80	68.33	68.83	68.68
toluene	CH_3	21.46	21.46	20.99	21.10	21.50	21.50	
	C(*i*)	137.89	138.48	137.35	137.91	138.90	138.85	
	CH(*o*)	129.07	129.76	128.88	129.33	129.94	129.91	
	CH(*m*)	128.26	129.03	128.18	128.56	129.23	129.20	
	CH(*p*)	125.33	126.12	125.29	125.68	126.28	126.29	
triethylamine	CH_3	11.61	12.49	11.74	12.35	12.38	11.09	9.07
	CH_2	46.25	47.07	45.74	46.77	47.10	46.96	47.19

[a] See footnotes for Table 1. [b] $^2J_{PC}$ = 3 Hz. [c] Reference material; see text.

*Reprinted with permission from J. Org. Chem. 1997, **62**, 7512-7515*

© 1997 American Chemical Society

NMR Formulae

Quantity	Formula (bold face = vectors)	Definitions (SI units) (see SI section for constants and units)
Magnetic Field Magnetic Force	$\boldsymbol{B} = \mu_o\ \boldsymbol{H}$ $\boldsymbol{F} = Q\ \boldsymbol{v}\times\boldsymbol{B}$	$\boldsymbol{B}$ = magn. flux density, magn. induction (T) $\boldsymbol{H}$ = magn. field strength (A m^{-1}) μ_o = permeability of vacuum ($4\pi\times10^{-7}$ H m^{-1}) Q = elec. charge (C); v = velocity (m/s)
Nuclear Spin Spin Angular Mom. Magn. Moment	$\boldsymbol{I}$ $\hbar\ m_I$ $\boldsymbol{\mu}_I = \gamma_I \hbar\ \boldsymbol{I} = g_I \beta_N\ \boldsymbol{I}$	γ = magnetogyric ratio (rad s^{-1} T^{-1}); $\hbar = h/2\pi$ $\beta_N = \mu_B$ (nuclear magneton); g_I = nuclear g factor m_I = quantum no. ($-I$, $-I$+1, ...+I)
Zeeman Interaction Larmor Freq. Nutation Vector	$\mathrm{H} = -\boldsymbol{\mu}_I \cdot \boldsymbol{B}_0$, $E = -m_I\ \gamma_I\ \hbar\ B_0$ $\omega_0 = \gamma_I B_0$, $\nu_0 = \nu_I\ B_0$ $\boldsymbol{\omega} = -\gamma_I\ \boldsymbol{B}$	ω in rad s^{-1}, ν in Hz ($\Delta m_I = \pm1$), $\nu = \gamma/2\pi$ (clockwise precession in lab frame for $\gamma > 0$)
Boltzmann Pop. Diff. Equil. Magn.	$\Delta N/N \sim \gamma_I\ \hbar/2kT\ (\Delta m_I = \pm1)$ $M_0 = B_0\ [N\gamma_I^2\hbar^2\ I(I+1)\ /\ 3kT]$	N = number of nuclei with spin I T = temperature (K)
Rotating Frame (r.f.) and residual field	$\gamma\ \Delta\boldsymbol{B}_0 = \gamma\ \boldsymbol{B}_0 + \boldsymbol{\omega}_{\mathbf{r.f.}}$ $\boldsymbol{\Omega} = -\gamma\ \Delta\boldsymbol{B}_0 = \boldsymbol{\omega_0} - \boldsymbol{\omega}_{\mathbf{r.f.}}$	$\boldsymbol{\omega}_{\mathbf{r.f.}}$ = rot. frame vector (detector freq.) in direction $\boldsymbol{\omega_0}$ ($-z$ axis for $\gamma > 0$) $\Delta\boldsymbol{B}_0$ = residual field in r.f. $\boldsymbol{\Omega}$ = precession freq. in r.f. (clockwise in r.f. for $\omega_0 > \omega_{r.f.}$)
Effective RF Field Amplitude and Tilt Nutation	$\boldsymbol{\omega}_1 = -\gamma\ \boldsymbol{B}_1$, $\boldsymbol{B}_{\mathbf{eff}} = \boldsymbol{B}_1 + \Delta\boldsymbol{B}_0$ $B_{\mathrm{eff}} = [B_1^2 + \Delta B_0^2]^{1/2}$, $\tan\theta = \Delta B_0/B_1$ $\boldsymbol{\beta}_{\mathbf{eff}}$ (in rad) $= -\gamma\ \boldsymbol{B}_{\mathbf{eff}}\ \tau_p$ $\nu_{B_{\mathrm{eff}}}$ (in Hz) $= 1/(4\tau_{90})$	$\boldsymbol{B}_1$ = RF field vector in xy plane; nutation is ccw around $\boldsymbol{\omega}_{\mathbf{eff}} = -\gamma\ \boldsymbol{B}_{\mathbf{eff}}$; θ = tilt angle between $\boldsymbol{B}_{\mathbf{eff}}$ and xy-plane; for $\Delta B_0/B_1 < 0.1$: $\theta < 6°$, $B_{\mathrm{eff}} \approx B_1$ τ_p = RF pulse width (s); τ_{90} = 90° pulse
Optimum flip angle	$\cos\beta_{\mathrm{opt}} = \exp(-\mathrm{TR}/T_1)$	TR = pulse repetition time
Relaxation rates	spin-lattice: $R_1 = 1/T_1$ spin-spin: $R_2 = 1/T_2 = \pi\Delta\nu_o$	$\Delta\nu_o$ = natural Lorentzian linewidth at half-height
Bulk Susceptibility Correction	for cylindrical samples with external ref. in coaxial capillary $\delta_{\mathrm{corr}} = \delta_{\mathrm{obs}} + C\ (\chi_{\mathrm{ref}} - \chi_{\mathrm{sample}})$	$C = +2\pi/3$ (tube perpendicular to B_0) $C = -4\pi/3$ (tube parallel to B_0)
Spin-echo amplitude in constant B_0 gradient	$M(2\ \tau) =$ $M_0\ \exp[-2\ \tau/T_2 - (2/3)(\gamma G)^2 D\tau^3]$	90-τ-180-τ Hahn echo with gradient G D = diffusion coeff. in gradient direction
Spin-echo attenuation in PFG-SE experiment	$\ln\ (S_{\mathrm{echo}}\ /\ S_0) = -bD$ $b = (\gamma\delta G)^2(\Delta - \delta/3)$	G = B_0 gradient pulse amplitude (T/m) δ = pulse width; Δ = pulse spacing
Rotational Correlation Time	Stokes-Einstein Relation $\tau_c = (4\pi\eta\ r^3)\ /\ (3kT)$	τ_c = rot. correlation time for isotropic tumbling η = viscosity; r = molecular radius (sphere)
Nuclear Oberhauser Enhancement	$M_S\{I\}/M_S(0) = 1 + 0.5(\gamma_I/\gamma_S)(R_1^{IS}/R_1^S)$ (extreme narrowing; $\omega_S\tau_C << 1$)	enhancement of spin S due to continuous irradiation of spin I; R_1^{IS} = dipolar relaxation of S via I; R_1^S = relaxation of S via all mechanisms
Polarization Transfer	$M_S\{PT\}/M_S(0) = \gamma_I/\gamma_S$	PT from I to S via J_{IS}
Lorentzian Lineshape	$a(\omega) = R_2\ /\ [R_2^2 + \Delta\omega^2]$ $d(\omega) = \Delta\omega\ /\ [R_2^2 + \Delta\omega^2]$	$a(\omega)$, $d(\omega)$ = absorption, dispersion signals $\Delta\omega = \omega - \boldsymbol{\Omega}$

NMR Formulae

NMR Relaxation

Mechanisms (isotropic tumbling, SI units)	**Remarks**
Intramolecular Heteronuclear Dipole-Dipole Spin I relaxed by Spin S $R_1^I = E_{IS}\, r_{IS}^{-6}\, [(1/12)J_0(\omega_I - \omega_S) + (3/2)J_1(\omega_I) + (3/4)J_2(\omega_I + \omega_S)]$ $R_2^I = E_{IS}\, r_{IS}^{-6}\, [(1/6)J_0(0) + (1/24)J_0(\omega_I - \omega_S) + (3/4)J_1(\omega_I) + (3/2)J_1(\omega_S) + (3/8)J_2(\omega_I + \omega_S)]$ where $E_{IS} = (\mu_0/4\pi)^2\, (\gamma_I\, \gamma_S\, \hbar)^2\, S(S+1)$ Extreme narrowing: $R_1^I = (4/3)\, E_{IS}\, r_{IS}^{-6}\, \tau_c\ (\omega\tau_c << 1)$ For several spins S: use $\sum r_{IS}^{-6}$ NB: $T_1^I = 1/R_1^I$ only when S is saturated	Factor $(\mu_0/4\pi) = 10^{-7}$ is required for conversion from cgs-Gauss units to MKSA (SI) units. Spectral Densities for random isotropic rotation $J_q(\omega) = C_q\, [\tau_c/(1 + \omega^2\tau_c^2)]$ $(q = 0,1,2)$ $C_0 = 24/15;\ C_1 = 4/15;\ C_2 = 16/15$ extreme narrowing: $J_q(\omega) = C_q\, \tau_c$
Intramolecular Homonuclear Dipole-Dipole Spin I_k relaxed by Spin I_1 $R_1^I = E_I\, r_{kl}^{-6}\, (3/2)\, [J_1(\omega_I) + J_2(2\omega_I)]$ $R_{1\rho}^I = E_I\, r_{kl}^{-6}\, [(3/8)J_0(\omega_1) + (15/4)J_1(\omega_I) + (3/8)J_2(2\omega_I)]$ $R_2^I = E_I\, r_{kl}^{-6}\, [(3/8)J_0(0) + (15/4)J_1(\omega_I) + (3/8)J_2(2\omega_I)]$ where $E_I = (\mu_0/4\pi)^2\, \gamma_I^4\, \hbar^2\, I(I+1)$ Extreme narrowing: $R_1^I = R_2^I = 2\, E_I\, r_{kl}^{-6}\, \tau_c\ (\omega\tau_c << 1)$ For several spins I: use $\sum r_{kl}^{-6}$	
Intermolecular Heteronuclear Dipole-Dipole Spin I on mol. A relaxed by Spin S on mol. B $(\omega\tau_C << 1)$ $R_1^I = 16\pi\, c_S\, E_{IS} / (27\, r_{IS}\, D_{trans})$ (pair distribution function = step function)	$E_{IS} = (\mu_0/4\pi)^2\, (\gamma_I\, \gamma_S\, \hbar)^2\, S(S+1)$ c_S = conc. of spins S r_{IS} = distance of closest approach $D_{trans} = (D_A + D_B)/2$
Intermolecular Homonuclear Dipole-Dipole Spin I on mol. A relaxed by Spin I on mol. B $(\omega\tau_C << 1)$ $R_1^I = 8\pi c_I\, E_I / (9\, r_{II}\, D_{trans})$ also found in the literature is: $R_1^I = (4\pi/3)\, c_I\, E_I\, (\tau/r_{II}^3)\, [1 + (2r_{II}^2/5\, D_{trans}\, \tau)]$	$E_I = (\mu_0/4\pi)^2\, \gamma_I^4\, \hbar^2\, I(I+1)$ c_I = conc. of spins I r_{II} = distance of closest approach τ = mol. jump time

Spherical Harmonics

Spherical harmonics up to rank 2 expressed in polar and orthogonal Cartesian coordinates

$Y_{0,0}$	$=$	$\sqrt{\frac{1}{4\pi}}$		
$Y_{1,0}$	$=$	$\sqrt{\frac{3}{4\pi}}\cos\theta$	$=$	$\sqrt{\frac{3}{4\pi}}\frac{z}{r}$
$Y_{1,\pm1}$	$=$	$\mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\varphi}$	$=$	$\mp\sqrt{\frac{3}{8\pi}}\frac{x \pm iy}{r}$
$Y_{2,0}$	$=$	$\sqrt{\frac{5}{16\pi}}\ (3\cos^2\theta - 1)$	$=$	$\sqrt{\frac{5}{16\pi}}\frac{2z^2 - x^2 - y^2}{r^2}$
$Y_{2,\pm1}$	$=$	$\mp\sqrt{\frac{15}{8\pi}}\cos\theta\ sin\theta\ e^{\pm i\varphi}$	$=$	$\mp\sqrt{\frac{15}{8\pi}}\frac{(x \pm iy)z}{r^2}$
$Y_{2,\pm2}$	$=$	$\sqrt{\frac{15}{32\pi}}\ \sin^2\theta\ e^{\pm 2i\varphi}$	$=$	$\sqrt{\frac{15}{32\pi}}\frac{(x \pm iy)^2}{r^2}$

NMR Formulae

Mechanisms (isotropic tumbling, SI units)	**Remarks**
Chemical Shift Anisotropy (CSA) molecular tumbling modulates the interaction of the chem. shift tensor with the B_0 field. $R_1 = (2/5)\ E_{CSA}\ [\tau_c / (1 + \omega^2\tau_c^2)]$ $R_2 = (1/90)\ E_{CSA}\ \{8\tau_c + [6\tau_c + (1 + \omega^2\tau_c^2)]\}$	predominant relaxation mech. for non-protonated X nuclei $E_{CSA} = \gamma^2\ B_0^2\ \Delta\sigma^2$ $\Delta\sigma = \sigma_\perp - \sigma_\parallel$ (in ppm) (assuming axial symmetry of tensor)
Quadrupole Relaxation ($I > 1/2$) $R_1 = R_2 = (3/40)\ C_i\ [1 + \eta^2/3]\ C_{QF}^2\ \tau_c \quad (\omega\tau_c << 1)$	$C_i = (2I + 3) / [I^2(2I - 1)]$ $C_{QF} = e^2\ Q\ q_{zz} / \hbar$ = quadrupolar coupling in Hz; η = asymmetry param.
Spin-Rotation Interaction (SR) Relaxation arises from the interaction of the nuclear spin with magnetic fields generated by the rotation of a molecular magnetic moment modulated by molecular collisions: $\left(\frac{1}{T_1}\right)_{SR} = \frac{2\ I_i\ kT}{3\ \hbar^2}\ C_{eff}^2\ \tau_J$ I_i = moment of inertia of the molecule C_{eff} = effective spin-rotational coupling constant τ_J = angular momentum correlation time With $\tau_c \cdot \tau_J = \frac{I_i}{6kT}$, we can introduce the reorientational correlation time and we obtain: $\left(\frac{1}{T_1}\right)_{SR} = \frac{I_i^2}{9\ \hbar^2}\ C_{eff}^2 \cdot \frac{1}{\tau_c}$	
Scalar Coupling (SC) This relaxation mechanism can occur if the nucleus I in question is scalar coupled (with coupling constant J) to a second spin ($S \geqq ½$) and the coupling is modulated by either chemical exchange (**SC relaxation of the first kind**) or the relaxation of spin S, e.g. if $S > ½$, (**SC relaxation of the second kind**). In this case spin splittings disappear and single lines are observed. $\left(\frac{1}{T_1}\right)_{SC} = \frac{8\pi^2\ J^2\ S\ (S+1)}{3}\ \left[\frac{\tau_{SC}}{1 + (\omega_I - \omega_S)^2\ \tau_{SC}^2}\right]$ $\left(\frac{1}{T_2}\right)_{SC} = \frac{4\pi^2\ J^2\ S\ (S+1)}{3}\ \left[\tau_{SC} + \frac{\tau_{SC}}{1 + (\omega_I - \omega_S)^2\ \tau_{SC}^2}\right]$ τ_{SC} = τ_e, if exchange time $\tau_e \ll T_1$ of either spin (first kind) τ_{SC} = T_1^S (the relaxation time of spin S) if $T_1^S \ll \tau_e$, $1/2\pi J$ (second kind) ω_I and ω_S are the resonance of I and S at the magnetic field in which $\left(\frac{1}{T_{1,2}}\right)_{SC}$ is measured.	